(12) INTERNATIONAL APPLICATION PUBLISHED UNDER THE PATENT COOPERATION TREATY (PCT)

(19) World Intellectual Property Organization
International Bureau

(43) International Publication Date
30 November 2000 (30.11.2000)

PCT

(10) International Publication Number
WO 00/71980 A1

(51) International Patent Classification[7]: G01J 3/28, G01N 21/27

(21) International Application Number: PCT/CA00/00583

(22) International Filing Date: 23 May 2000 (23.05.2000)

(25) Filing Language: English

(26) Publication Language: English

(30) Priority Data:
2,273,132 21 May 1999 (21.05.1999) CA

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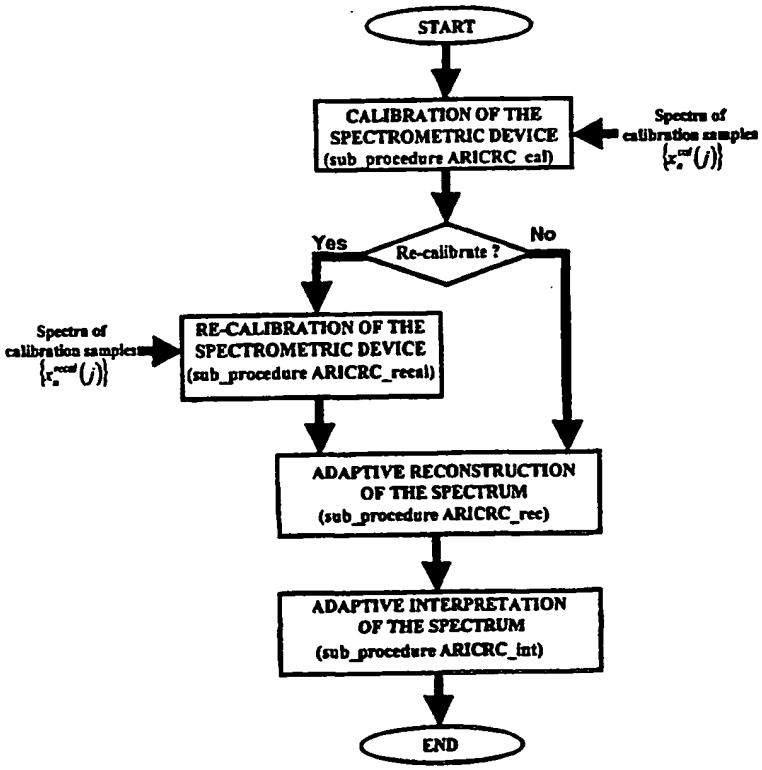
(81) Designated States *(national)*: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO,

[Continued on next page]

(54) Title: METHOD AND SYSTEM FOR ADAPTIVE INTERPRETATION OF SPECTROMETRIC DATA COMBINED WITH CONTINUAL RE-CALIBRATION



(57) Abstract: A method for adaptive reconstruction and interpretation of spectra combined with re-calibration of a device providing spectrometric data, consist in carrying out an automatic calibration using the external reference light spectrum and its corresponding digital reference data stored in the internal memory of the device. The continual re-calibration procedure allows for automatic adaptation of the values of the coefficients in a reconstruction sub-procedure as well as the estimation of the values of the coefficients in an interpretation sub-procedure on the bases of a current shape of spectrometric data.

WO 00/71980 A1

NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW.

(84) **Designated States** *(regional)*: ARIPO patent (GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW), Eurasian patent (AM, AZ, BY, KG, KZ, MD, RU, TJ, TM), European patent (AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE), OAPI patent (BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG).

Published:

— *With international search report.*

— *Before the expiration of the time limit for amending the claims and to be republished in the event of receipt of amendments.*

For two-letter codes and other abbreviations, refer to the "Guidance Notes on Codes and Abbreviations" appearing at the beginning of each regular issue of the PCT Gazette.

Method and system for adaptive interpretation of spectrometric data combined with continual re-calibration

Field of Invention

This invention relates generally to light-spectrum-measurement and more specifically to compact systems for light-spectrum-measurement for portability and for *in situ* applications.

Background of the invention

Spectroscopy is an analytic technique concerned with the measurement characterization of the interaction of radiant energy with matter, including the instruments designed for this purpose, called *spectrometers*, and corresponding means of the interpretation of the interaction both at the fundamental level and for practical analysis. The distribution of radiant energy, absorbed or emitted by a sample of a substance under study, is called its *spectrum*. Interpretation of spectra provides fundamental information at atomic and molecular energy levels, the distribution of species within those levels, the nature of processes involving change from one level to another, molecular geometries, chemical bonding, and interaction of molecules in solution. At the practical level, comparisons of spectra provide a basis for the determination of qualitative chemical composition and chemical structure, and for quantitative chemical analysis.

The spectra to be measured have two common features: they are non-negative, and they may be decomposed into relatively flat regions and peaks of various widths. The interpretation of the data representative of those spectra obtained by means of spectrometers, very frequently involves estimation of some parameters of the peaks, viz.: of their positions and magnitudes (i.e. areas or heights). The parameters of the peaks are used, in particular, for qualitative and quantitative analysis of complex chemical substances:

- the positions of peaks are used for identification of the compounds which are present in a sample of the substance under study;

- the magnitudes of peaks are used for estimation of the concentrations of the identified compounds.

The estimation of the parameters of spectrometric peaks directly from the acquired spectrometric data is in many practically important cases problematic because of:

- instrumental imperfections of the spectrometer, and
- some natural phenomena in a sample of the substance under study.

The imperfections of the spectrometer produce blurring of peaks and noise-type disturbances in the data representative of the measured spectrum. On the other hand, some quantum phenomena in the substance enlarge considerably the width of peaks. Both instrumental blurring and natural enlargement of peaks may contribute to their overlapping and fusion, making impossible their proper identification. Different algorithms of deconvolution have been developed for reducing instrumental blurring; a review of these algorithms may be found in Jansson P. A. (Ed.) : *Deconvolution with Applications in Spectroscopy*. Academic Press, 1984 and Morawski R. Z., Szczeciń ski L., Barwicz A.: "Deconvolution Algorithms for Instrumental Applications - A Comparative Study", *J. Chemometrics,* 1995, Vol. 9, pp. 3-20. These algorithms are designed and assessed using the criteria of the quality of deconvolution, which is not specific of spectrometry; e.g. the root-mean-square errors of approximation. Consequently, the estimates of the magnitudes determined on the basis of the results of deconvolution may turn out to be very poor. On the other hand, the curve-fitting algorithms may be very inefficient if not provided with a good initial guess of the sought-for estimates. These two observations inspired independently many researchers to subsequently use a deconvolution algorithm for estimation of the positions and a curve-fitting algorithm for estimation of magnitudes of spectral peaks.

Both the algorithms of spectrum reconstruction and the algorithms of spectrum parameter estimation require considerable amount of information on the mathematical model of the spectrometric data. This information is acquired during initial calibration of the spectrometer.

The numerical algorithms necessary for calibration of the spectrometer, reconstruction of the spectrum and estimation of its parameters are available in many software libraries, e.g. in some MATLAB Toolboxes, including specialized libraries dedicated to processing of spectrometric data, e.g. GRAMS/32 of Galactic Industries. In the patent domain, there is only a partial methodology for spectrum deconvolution, e.g. the US Patent No.5 247 175, issued September 21, 1993, in the name of Alan E. Schoen *et al.*, entitled *Method and Apparatus for the Deconvolution of Unresolved Data* as well the US Patent No.4 941 101, issued July 10, 1990, in the name of Paul B. Crilly, entitled *Method for Analyzing Chromatograms* specific to the domain of chromatography. On the other hand, there is a good example of a complete methodology of spectrometric data interpretation – c.f. the US Patent No. 5,991,023, issued November 23, 1999, in the name of R. Z Morawski et al., entitled *Method of interpreting spectrometric data.*

However, in all the above-listed references, none of them offers full support for the methodology of on-line continual re-calibration and adaptive spectrometric data interpretation, mainly due to the fact that there are no closed procedures of such re-calibration and adaptive interpretation.

The demand for an increased-resolution and a self calibrated spectrometric device comes from everyday practice. The US Patent No. 5040889, issued August 21,1991, in the name of Thomas J. Keane, entitled *Spectrometer with Combined Visible and Ultraviolet Sample Illumination*, describes a spectrometer with an automatic calibration of the photodetectors, based on the use of a pivotable standard white sample positioned in the path of the light and controlled by a computer system. A calibration factor is computed and recalculated for each photodetector whenever the temperature changes within the spectrometer, and then used to multiply the output signal of the photodetectors. However, this is a partial static calibration, since it corrects only the effect of the photodetectors and doesn't take into account the effect of the dynamical errors introduced by the light diffraction element and the slits. Thus, there is a need for another dynamic calibration procedure to eliminate these instrumental errors and enhance the spectrum resolution. In the fields of telecommunications, especially for optical performance

monitoring of networks, there is a need for a spectrometric device, which must be compact, operating under a broader range of environmental conditions and more particularly self-calibrating. In Miller C., Pelz L.: "Fabry-Perot Tunable Filters Improve Optical Channel Analyzer Performance", *Lightwave*, March 1999, Vol. 16, No. 3, a card mounted optical channel analyzer performance, based on the use of a fiber Fabry-Perot tunable filter, is described. This device uses an optical switch to alternately scan the light spectrum (coming for example from a DWDM system) and a known wavelengths reference source. This latter is used for the continual calibration of the device in order to correct the thermal drifts, the nonlinearities of the actuator and the voltage variations. A deconvolution algorithm is also used to remove the effects of the tunable filter spectral response in order to enhance the resolution of the measured light spectrum. The major drawback of this device is that it measures one wavelength or path length difference at a time, thus necessitating a long time to process all the optical channels. Thus, a need remains for a low-cost miniaturized spectrometric device, self-calibrated, with a spectral resolution comparable to that of conventional optical spectrum analyzer, and capable of determining the spectral signature of a wide variety of light spectra *in situ*.

In the domain of spectroscopy, the demand for an adaptive reconstruction and interpretation procedures combined with a continual re-calibration is generated by the need for a spectrometric device that can be compact, autonomous with a higher degree of reliability, self-calibrated, operating under a broader range of environmental conditions, and be cost-effective for wide deployment. The main objective of the invention is to respond to this demand.

Object of Invention

It is an object of this invention to provide a method for adaptive interpretation of spectra on the basis of spectrometric data.

It is an object of this invention to provide a method for calibration and continual re-calibration of integrated spectrometric devices allowing for miniaturization and low-cost mass production of micro-optical spectrum analyzers.

Summary of the invention

It is an object of this invention to provide a procedure for interpretation of spectrometric data, representative of a sample of the substance under study, comprising the steps of:

- initial calibration of the spectrometric device;
- continual re-calibration of the spectrometric device
- adaptive reconstruction of the spectrum under study; and
- adaptive interpretation of the spectrum under study.

The invention also provides a method for calibration and continual re-calibration of the spectrometric device, i.e. for identification of a numerical relation between the measurement results produced by this spectrometric device and established measurement standards of spectrum.

The invention also provides a method for continual re-calibration of the spectrometric device allowing for automatic adaptation of the method to possible variation of the instrumental imperfections and a shape of spectrometric data due to the aging of the device and/or thermal drifts and nonlinearities of the detector.

The invention also provides a method for numerical adaptive reconstruction of the spectrum under study, combined with the continual re-calibration of the spectrometric device, i.e. for partial elimination of the effects of noise and blur corrupting the spectrometric data.

The invention also provides a method for numerical adaptive interpretation, i.e. estimation of the positions and magnitudes of peaks the spectrum of the light is composed of.

According to the invention, the calibration of the spectrometer is accomplished using an auxiliary light whose spectrum is assumed to be known and representative of the spectra to be measured in the series of experiments following the calibration. The result of calibration has the form of two operators defining the following numerical algorithms:

- an algorithm for simulation of the spectrometric data, given the spectrum to be measured (operator of projection $\mathscr{S}$);
- an algorithm for estimation of the spectrum, given the data (operator of reconstruction $\mathscr{R}$).

The first algorithm is an algorithm of model identification including choice or estimation of the structural parameters of the model and estimation of its functional parameters. The second algorithm is an algorithm of deconvolution, or an algorithm of generalized deconvolution, or an algorithm for numerically solving the first-kind integral equations.

According to the invention, the continual re-calibration of the spectrometer is accomplished using an external reference light spectrum and the digital reference data representing this reference light, stored in a computer or an internal memory, when available, of the spectrometric device. The re-calibration of the device is aimed at updating the parameters of the above mentioned operators.

According to the invention, the processing of the data representative of the light under study is comprising two main operations:

- estimation of the unknown spectrum or its idealized version on the basis of the acquired spectrometric data, using the operator of reconstruction $\mathscr{R}$;
- estimation of the parameters of this spectrum on the basis of the acquired spectrometric data, using the operator of projection $\mathscr{S}$ and an algorithm of curve fitting.

The method of adaptive interpretation of spectrometric data is useful for providing the quality light-spectrum measurement especially in the case of miniature integrated intelligent spectrometric devices. When combined with automatic recalibration continually or at intervals the spectrometric device keeps optimum performance, in particular, for telecommunication applications.

The proposed method allows for automatic calibration of especially miniature integrated spectrometric devices during a manufacturing process and absent physical

tuning of individual devices. The calibration will compensate for many forms of fabrication discrepancies without modification of the physical devices.

As the consequence, it contributes to a low-cost flexible quality light-spectrum-measurement solution, especially on-chip light spectrum measurement, which may be easily adapted to very diversified applications via customization of the specific set of algorithms.

Brief description of the drawings

Exemplary embodiment of the invention will now be described in conjunction with the drawings in which:

Fig. 1. presents an exemplary measuring system;

Fig 2. presents the flow diagram of the procedures of adaptive reconstruction and interpretation

a) the procedure AI-RC,

b) the sub-procedure AI-RC_cal,

c) the sub-procedure AI-RC_recal,

d) the sub-procedure AI-RC_rec,

e) the sub-procedure AI-RC_int;

Fig. 3. presents the exemplary measuring system;

Fig. 4. presents the spectrum of the test sample:

a) real spectrum $x(\lambda)$,

b) the test data $\{\tilde{y}_n\}$;

Fig. 5. presents the spectrum of the sample used for calibration:

a) real spectrum $x^{cal}(\lambda)$,

b) the data $\{\tilde{y}_n^{cal}\}$;

Fig. 6. presents the output of:

a) the rational filter,

b) the spline-based Kalman filter;

Fig. 7. presents the final result of spectrometric data interpretation;

Fig. 8. presents the exemplary measuring system – MM microOSA;

Fig. 9. shows possible applications of MM microOSA™ in Dense Wavelength Division Multiplexing (DWDM) system;

Fig. 10. presents the spectrum of the test light:

a) the idealized spectrum $s(\lambda)$ of the light at the input of the DWDM transmitter,

b) the test data $\{\tilde{y}_n\}$;

Fig. 11. presents the emission spectrum of the laser; and,

Fig. 12. illustrates the final result of adaptive reconstruction and interpretation of telecommunication data.

Detailed Description of the Invention

The procedure of adaptive reconstruction combined with continual re-calibration of a device providing spectrometric data and adaptive interpretation of spectra (AI-RC) is designed for a measuring system, for example the system shown in Fig.1, comprising:

- a spectrometric device in the form of a spectrometer or its essential part, in the form of a micro-optical spectrum analyzer converting an optical signal carrying the information on the measured spectrum into a digital code representing this spectrum;
- a processing means for processing the digital representation, in the form of a general-purpose computer, a microprocessor, a general-purpose digital signal processor, or an application-specific digital signal processor; and
- other functional elements necessary for measuring the spectrum of light.

The following notation is used for the description of the procedure AI-RC:

λ - wavelength; $\lambda \in [\lambda_{\min}, \lambda_{\max}]$;

N - number of data acquired by a spectrometric apparatus;

$\Delta\lambda$ - step of wavelength discretization; $\Delta\lambda = (\lambda_{\max} - \lambda_{\min})/(N-1)$;

λ_n - n-th datum acquired by the spectrometric apparatus; $\lambda_n = \lambda_{\min} + (n-1)\Delta\lambda$ for $n = 1,...,N$;

$x(\lambda)$ - real spectrum of a light under study;

$\mathbf{l}$ - a vector of positions of peaks within the spectrum $x(\lambda)$ is composed of;

$\mathbf{l} = [l_1\ l_2\ \ldots\ l_K]^T$;

$\hat{\mathbf{l}}$ - an estimate of $\mathbf{l}$;

$\mathbf{a}$ - a vector of magnitudes of peaks within the spectrum $x(\lambda)$ is composed of;

$\mathbf{a} = [a_1\ a_2\ \ldots\ a_K]^T$;

$\hat{\mathbf{a}}$ - an estimate of $\mathbf{a}$;

$s(\lambda;\mathbf{l},\mathbf{a})$ - an idealized spectrum of light under study and, in the preferred embodiment, assumed to have the form:

$$s(\lambda;\mathbf{l},\mathbf{a}) = \sum_{k=1}^{K} a_k v_s(\lambda, l_k)$$

where $v_s(\lambda, l)$ is an isolated, normalized peak in $s(\lambda;\mathbf{l},\mathbf{a})$, whose maximum is located at $\lambda = l$;

$$\int_{-\infty}^{+\infty} v_s(\lambda, l)\, d\lambda = 1 \text{ for } l \in [\lambda_{\min}, \lambda_{\max}];$$

$\{\tilde{y}_n\}$ - spectrometric data representative of $x(\lambda)$, acquired by means of the spectrometric apparatus;

$$\{\tilde{y}_n\} \equiv \{\tilde{y}_n \mid n = 1,\ldots,N\};$$

$x^{cal}(\lambda)$ - a real spectrum of light used for calibration of the spectrometric device;

$s(\lambda;\mathbf{l}^{cal},\mathbf{a}^{cal})$ - an idealized spectrum of light used for calibration of the spectrometric device;

$\{\tilde{y}_n^{cal}\}$ - the spectrometric data, representative of $x^{cal}(\lambda)$ used for calibration of the spectrometric device;

$$\{\tilde{y}_n^{cal}\} \equiv \{\tilde{y}_n^{cal} \mid n = 1,\ldots,N^{cal}\};$$

$x^{recal}(\lambda)$ - the real spectrum of an external reference light used for the re-calibration of the spectrometric device;

$\{\tilde{y}_n^{recal}\}$ - the spectrometric data measured using the spectrometric device, representative of $x^{recal}(\lambda)$ used for the re-calibration of this device;

$\{\tilde{y}_n^{recal}\} \equiv \{\tilde{y}_n^{recal} \mid n = 1,\ldots,N^{recal}\}$;

$s(\lambda;\mathbf{l}^{recal},\mathbf{a}^{recal})$ - an idealized spectrum of a light used for the re-calibration of the spectrometric device;

G - an operator (transform) of projection mapping the idealized spectrum $s(\lambda;\mathbf{l},\mathbf{a})$ into the space of the data:

$$\{\hat{x}_n\}=G\ [s(\lambda;\mathbf{l},\mathbf{a});\mathbf{p}_G\ ]$$

where $\mathbf{p}_G$ is a vector or matrix of the parameters of the operator G, to be determined during calibration of the spectrometric device; $\mathbf{p}_G = [p_{G,1}\, p_{G,2} \ldots]^T$ or:

$$\mathbf{p}_G = \begin{bmatrix} p_{G,1,1} & p_{G,1,2} & \cdots \\ p_{G,2,1} & p_{G,2,2} & \cdots \\ \vdots & \vdots & \ddots \end{bmatrix}$$

R - an operator (transform) of reconstruction and interpretation:

$$R = R^r \circ R^i$$

R^r - an operator (transform) of reconstruction, in the form of a generalized deconvolution method, for transforming the data $\{\tilde{y}_n\}$ into an estimate $\{\hat{x}_n\}$ of $x(\lambda)$:

$$\{\hat{x}_n\}=R^r[\{\tilde{y}_n\};\mathbf{p}_{R^r}]$$

where $\mathbf{p}_{R^r} = [p_{R^r,1}\, p_{R^r,2} \ldots]^T$ are parameters of the operator R^r including regularization parameters for determination during calibration of the spectrometric device.

R^i - an operator (transform) of interpretation, in the form of a generalized deconvolution method, for transforming the data $\{x_n\}$ into an estimate $\hat{s}(\lambda)$ of $s(\lambda;\mathbf{l},\mathbf{a})$:

$$\hat{s}(\lambda)=R^i[\{x_n\};\mathbf{p}_{R^i}]$$

where $\mathbf{p}_{R^i} = [p_{R^i,1}\, p_{R^i,2} \ldots]^T$ are parameters of the operator R^i including regularization parameters for determination during calibration.

2. Functional specification of a preferred embodiment of the invention

2.1. General specification of the procedure AI-RC

The main objective of the procedure AI-RC is estimation of the positions **l** and magnitudes **a** of the peaks contained in a spectrum of a light under study $x(\lambda)$ on the basis of the acquired spectrometric data $\{\tilde{y}_n\}$. The feasibility of this operation is critically conditioned by an auxiliary operation on the reference data $\{\tilde{y}_n^{cal}\}$ and corresponding reference spectrum $x^{cal}(\lambda)$, referred to as *calibration of the spectrometric device*. This operation is aimed at the acquisition of information relating to a mathematical model of a relationship between spectrometric data and idealized spectrometric data known to be measured, which underlies the method chosen for estimation of the parameters **l** and **a**. Although calibration does not necessarily immediately precede processing of each sequence or sample of spectrometric data $\{\tilde{y}_n\}$, preferably valid calibration results are always available during spectral processing.

The main difficulty relating to estimation of the positions **l** and magnitudes **a** of spectrometric peaks within a sensed spectrum is implied by blurring of those peaks, caused by physical phenomena in a sample, and by blurring of their representations in the data $\{\tilde{y}_n\}$, caused by an imperfect spectrometric apparatus. This difficulty is overcome in the procedure AI-RC through application of a series of steps for adaptive reconstruction and adaptive interpretation of an idealized – hypothetical - spectrum $s(\lambda;\mathbf{l},\mathbf{a})$ in order to correct the sensed data to reduce both types of blurring; if $s(\lambda;\mathbf{l},\mathbf{a})$ is assumed to be an approximation of $x(\lambda)$, then only the instrumental blurring needs to be corrected.

In accordance with the above general functional specification, AI-RC is composed of the following broadly defined steps:

- initial calibration of the device providing the spectrometric data, *i.e.* of the spectrometric apparatus or of the spectrometric sensor or of the spectrometric transducer (the sub-procedure AI-RC_cal),
- continual re-calibration of that device on the basis of auxiliary reference data obtained by means of the device stimulated with the reference light (the sub-procedure AI-RC_recal),

- adaptive reconstruction of the spectrum under study $\{x_n\}$, i.e. estimation of this spectrum on the basis of the spectrometric data $\{\tilde{y}_n\}$ representative of the spectrum $\{x_n\}$ (the sub-procedure AI-RC_rec), and
- adaptive interpretation of the spectrum under study $\{x_n\}$ in the form of adaptive estimation of the positions $l_1, l_2, \ldots$ and magnitudes $a_1, a_2, \ldots$ of peaks this spectrum is composed of – on the basis of an estimate $\{\hat{x}_n\}$ of the real spectrum, obtained by means of the sub-procedure AI-RC_rec (the sub-procedure AI-RC_int).

2.2. Detailed specification of the sub-procedure AI-RC_cal

The sub-procedure AI-RC_cal comprises the following operations:

a) choosing the method for idealization of the spectrum, *i.e.* the form of peaks of the idealized spectrum $\{s_n\}$;

b) choosing the form of the operator R for reconstruction of the idealized spectrum: $\{\hat{s}_n\} = \mathsf{R}\,[\{\tilde{y}_n\}; \mathbf{p}_\mathsf{R}]$, where $\mathbf{p}_\mathsf{R}$ is a vector of the parameters;

c) choosing the rules for adaptation of the parameters $\mathbf{p}_\mathsf{R}$ to the selected features $F_1, F_2, \ldots$ of the spectrum under study $\{x_n\}$ or of the data $\{\tilde{y}_n\}$ – on the basis of the library of parameters $\left\{\mathbf{p}_\mathsf{R}^{(j)} \mid j = 1,\ldots,J\right\}$ to be determined during initial calibration, and updated during continual re-calibration;

d) choosing reference light signals for the initial calibration: $\left\{x_n^{cal}(j)\right\}$ and related $\left\{s_n^{cal}(j)\right\}$ for $j=1,\ldots,J$;

acquiring the data $\left\{\tilde{y}_n^{cal}\right\}$ representative of $\left\{x_n^{cal}(j)\right\}$ for $j=1,\ldots,J$;

e) pre-processing of the data $\left\{\tilde{y}_n^{cal}\right\}$ including the elimination of outliers, baseline subtraction, smoothing, acquiring *a priori* information for the operation 2.g (*e.g.* a pre-estimate of the variance of errors in the calibration data), normalization, *etc.*;

f) determination of the vectors of parameters $\mathbf{p}_\mathsf{R}^{(j)}$ – on the basis of the triplets: $\left\{\tilde{y}_n^{cal}(j)\right\}$ $\left\{x_n^{cal}(j)\right\}$ and $\left\{s_n^{cal}(j)\right\}$ for $j=1,\ldots,J$;

g) approximation of the relationship between the parameters $\mathbf{p}_R$ and the features $F_1, F_2, \ldots$ controlling the adaptation.

2.3. Detailed specification of the sub-procedure AI-RC_recal

The sub-procedure AI-RC_recal comprises the following operations:

a) choosing the reference light signals for re-calibration: $\{x_n^{recal}(j)\}$ and related $\{s_n^{recal}(j)\}$ for $j=1,\ldots,J$;

b) acquiring the data $\{\tilde{y}_n^{recal}\}$ representative of $\{x_n^{recal}(j)\}$ for $j=1,\ldots,J$;

c) pre-processing of the data $\{\tilde{y}_n^{recal}\}$ including elimination of outliers, baseline subtraction, smoothing, acquiring *a priori* information for the operation 3.d (*e.g.* a pre-estimate of the variance of errors in the calibration data), normalization, *etc.*;

d) updating of the vectors of parameters $\mathbf{p}_R^{(j)}$ on the basis of triplets: $\{\tilde{y}_n^{recal}(j)\}$, $\{x_n^{recal}(j)\}$ and $\{s_n^{recal}(j)\}$ for $j=1,\ldots,J$;

e) updating the approximation of the relationship between the parameters $\mathbf{p}_R$ and the features $F_1, F_2, \ldots$ controlling the adaptation.

2.4. Detailed specification of the sub-procedure AI-RC_rec

The sub-procedure AI-RC_rec comprises the following operations:

a) acquiring data $\{\tilde{y}_n\}$ representative of the spectrum under study $\{x_n\}$;

b) pre-processing of $\{\tilde{y}_n\}$ including elimination of outliers, baseline subtraction, smoothing, acquiring *a priori* information for the estimation of peak parameters in the form of a pre-estimate of the variance of errors in the data, acquiring *a priori* information for the reconstruction in the form of determination of apparatus fabrication imperfections on the basis of characteristics of measured spectrum $\{\tilde{y}_n\}$, ambient temperature sensed with a temperature sensor, and aging of working apparatus elements, normalization, etc.;

c) estimation of the spectrum under study $\{x_n\}$ on the basis of the data $\{\tilde{y}_n\}$, by means of the operator $\mathbf{R}^r$ with the parameters $\mathbf{p}_R$, being continuously adapted to the features of

3. An exemplary embodiment of the invention

Example 1

A particular version of the procedure AI-RC has been designed for a measuring system shown in Fig. 3 and including: the absorption mini spectrophotometer - model S1000 by Ocean Optics®; and a personal computer PC.

The following measurement parameters were selected both for calibration and for acquisition of the test data:

- the wavelength range: $\lambda_{\min} = 450nm, \lambda_{\max} = 675nm$;
- the number of data acquired by the spectrophotometer: $N = 1024$; and,
- the step of wavelength discretization: $\Delta\lambda = (\lambda_{\max} - \lambda_{\min})/(N-1) = 0.22nm$.

The test data were acquired for a standard holmium perchlorate solution sample; its real spectrum $x(\lambda)$ is shown in Fig. 4a. The parameters of this spectrum are the following:

- the vector of the positions of peaks:

$$\mathbf{l} = [452.2 \quad 468.2 \quad 473.1 \quad 485 \quad 537.3 \quad 541.3 \quad 543.7 \quad 639.8 \quad 644.2 \quad 652.2 \quad 656.4]^T$$

- the vector of the magnitudes of peaks:

$$\mathbf{a} = [1.17 \quad 0.19 \quad 0.2 \quad 0.461 \quad 0.988 \quad 0.41 \quad 0.297 \quad 0.821 \quad 0.406 \quad 0.246 \quad 0.263]^T$$

The idealized spectrum of a sample under study has been assumed to have the form:

$$s(\lambda;\mathbf{l},\mathbf{a}) = \sum_{k=1}^{11} a_k v_s(\lambda, l_k)$$

with the peaks defined by:

$$v_s(\lambda, l) = \delta(\lambda - l) \quad \text{for } l \in [\lambda_{\min}, \lambda_{\max}]$$

The set of data representative of $x(\lambda)$, acquired by means of the spectrophotometer, $\{\tilde{y}_n\} \equiv \{\tilde{y}_n \mid n = 1,...,1024\}$, is shown in Fig. 4b.

Calibration data have been acquired for the standard holmium oxide filter sample; its real spectrum $x^{cal}(\lambda)$ is shown in Fig. 5a. The parameters of this spectrum are the following:

- the vector of the positions of peaks:

$$\mathbf{l}^{cal} = [450.7 \quad 454.5 \quad 460.4 \quad 463.5 \quad 473.9 \quad 483.9 \quad 488.8 \quad 536.4 \quad 547.5 \quad 633.4 \quad 636.5 \quad 648.4]^T$$

;

- the vector of the magnitudes of peaks:

$$\mathbf{a}^{cal} = [0.486 \quad 0.799 \quad 0.949 \quad 0.58 \quad 0.125 \quad 0.117 \quad 0.114 \quad 0.284 \quad 0.106 \quad 0.129 \quad 0.149 \quad 0.109]^T$$

. The idealized spectrum of a sample used for calibration $s(\lambda;\mathbf{l}^{cal},\mathbf{a}^{cal})$ has been assumed to have the form:

$$s(\lambda;\mathbf{l}^{cal},\mathbf{a}^{cal}) = \sum_{k=1}^{12} a_k^{cal} v_s(\lambda, l_k^{cal})$$

The set of data representative of $x^{cal}(\lambda)$, acquired by means of the spectrophotometer, $\{\tilde{y}_n^{cal}\} \equiv \{\tilde{y}_n^{cal} \mid n = 1,...,1024\}$, is shown in Fig. 5b.

The chosen operator (transform) of projection, mapping the idealized spectrum $s(\lambda;\mathbf{l},\mathbf{a})$ into the space of the data:

$$\{\hat{y}_n\} = G\left[s(\lambda;\mathbf{l},\mathbf{a});\mathbf{p}_G\right]$$

has been defined by the following operations:

$$x(\lambda) = \exp\left[\int_{-\infty}^{+\infty} g_{xx}(\lambda-\lambda')\ln[s(\lambda';\mathbf{l},\mathbf{a})]\,d\lambda'\right]$$

$$y(\lambda) = \int_{-\infty}^{+\infty} g_{xy}(\lambda-\lambda')\,x(\lambda')\,d\lambda'$$

$$\hat{y}_n = y(\lambda_n) \text{ for } n = 1,...,N$$

The function $g_{xy}(\lambda)$ has been assumed to have the form of the Gauss function:

$$g_{xy}(\lambda) = \frac{1}{\sqrt{2\pi}\sigma_{xy}}\exp\left(-\frac{\lambda^2}{2\sigma_{xy}^2}\right)$$

Consequently, the vector of the parameters $\mathbf{p}_G$ of the operator G contains the discrete values of $g_{xx}(\lambda)$ and the parameter σ_{xy}.

The chosen operator (algorithm) of reconstruction, transforming the data $\{\tilde{y}_n\}$ into an estimate $\hat{s}(\lambda)$ of $s(\lambda;\mathbf{l},\mathbf{a})$,

$$\hat{s}(\lambda)=R\left[\{\tilde{y}_n\};\mathbf{p}_R\right]$$

is defined by in the following way:

a discrete estimate $\{\hat{x}_n\}$ of $x(\lambda)$ is found by means of the rational filter described by Szczeciń ski L.: "Méthodes non linéaires de reconstitution de signaux pour des applications spectrométriques", Ph. D. thesis, Université du Québec - Institut National de la Recherche Scientifique «Telecommunications», Montréal 1997. and applied to the data $\{\tilde{y}_n\}$;

- an estimate $\hat{s}(\lambda)$ of $s(\lambda;\mathbf{l},\mathbf{a})$ is computed by means of the adaptive rational filter as described in Wisniewski M. P., Morawski R. Z., Barwicz A., 1999, "An Adaptive Rational Filter For Interpretation of Spectrometric Data", to be published in *IEEE Trans. Instrum. & Meas.* applied to $\{\hat{x}_n\}$.

The vector $\mathbf{p}_{R'} = [p_{R',1}\ p_{R',2}\ \ldots]^T$ of the parameters of the operator R' contains the coefficients of the rational filter, as well as the discrete values of the function $g_{xx}(\lambda)$ as described in Ben Slima M., Szczecinski L., Massicotte D., Morawski R. Z., Barwicz A.: "Algorithmic Specification of a Specialized Processor for Spectrometric Applictions", *Proc. IEEE Instrum. & Meas. Technology Conf. (Ottawa, Canada, May 19-21, 1997)*, pp. 90-95 and in Ben Slima M., Morawski R. Z., Barwicz A.: "Kalman-filter-based Algorithms of Spectrophotometric Data Correction - Part II: Use of Splines for Approximation of Spectra", *IEEE Trans. Instrum. & Meas.*, Vol. 46, No. 3, June 1997, pp. 685-689.

The following operations are accomplished during the initial calibration:

- identification of the function $g_{xx}(\lambda)$, using an iterative algorithm as described by Jansson;
- estimation of the parameter σ_{xy} of the function $g_{xy}(\lambda)$ on the basis of a real spectrum $x^{cal}(\lambda)$ using an optimization algorithm; and
- estimation of coefficients of the rational filter using an optimization algorithm.

The following operations are accomplished during the continual re-calibration:

- updating coefficients of the rational filter using an optimization algorithm; and
- estimating coefficients of the adaptive rational filter using an optimization method and a shape of spectrometric data.

The exemplary results of spectrophotometric data interpretation, obtained by means of the described preferred embodiment are shown in Fig. 6a, Fig. 6b and Fig. 7.

The following errors are defined to evaluate the exactitude of the procedure AI-RC:

- relative root-mean-square error (RRMSE)

$$\partial_2^l = \frac{\|\hat{\mathbf{i}} - \mathbf{i}\|_2}{\|\mathbf{i}\|_2}, \quad \partial_2^a = \frac{\|\hat{\mathbf{a}} - \mathbf{a}\|_2}{\|\mathbf{a}\|_2}$$

- normalized maximum error (NME)

$$\partial_\infty^l = \frac{\|\hat{\mathbf{i}} - \mathbf{i}\|_\infty}{\|\mathbf{i}\|_\infty}, \quad \partial_\infty^a = \frac{\|\hat{\mathbf{a}} - \mathbf{a}\|_\infty}{\|\mathbf{a}\|_\infty}$$

The errors of estimation of positions and heights of peaks, are:

$$\partial_2^l = 0.0015, \quad \partial_\infty^l = 0.0024; \quad \partial_2^a = 0.20, \quad \partial_\infty^a = 0.23;$$

Example 2

An embodiment of AI-RC was designed for a measuring system which is represented by the integrated MM microOSA (*Optical Spectrum Analyser*) as shown in Fig. 8. The analyser is shown used for optical channel monitoring in DWDM networks in Fig. 9.

The following DWDM system parameters have been selected both for calibration and for acquisition of test data:

- number of optical channels : 81;
- wavelength range: $\lambda_{min} = 1530.77nm$, $\lambda_{max} = 1562.68nm$;
- channel spacing : $\Delta\lambda$ = 0.4 nm (50 GHz);
- laser sources with a known FWHM = 0.2 nm, where FWHM denotes Full Width at Half Maximum

The test data were acquired for a telecommunication bandwidth; its real spectrum $x(\lambda)$ is shown in Fig. 10a. The parameters of this spectrum are the following:

- the vector of the positions of peaks (carrier frequencies):

$$l_k = 1530.28 + (k-1)\,\Delta\lambda + dl_k \quad (k=1,\ldots,81),$$

where dl_k are realizations of identical independent random variables uniformly distributed in the interval [-0.05 nm;0.05 nm], *i.e.* $dl_k \propto U(-0.05, 0.05)$;

- the vector **a** of the heights of peaks, that are assumed to be realizations of identical independent random variables uniformly distributed in the interval [0.01 ; 1], *i.e.* $a_k \propto U(0.01, 1.0)$.

The adaptation of the MM μOSA for DWDM applications means that the model of the data takes on the form:

$$\{\tilde{y}_n\} = \left\{ g_{xy}(\lambda) * x(\lambda)\big|_{\lambda=\lambda_n} \right\} + \{\eta_n\} = \left\{ g_{xy}(\lambda) * g_{sx}(\lambda) * s(\lambda;\mathbf{l},\mathbf{a})\big|_{\lambda=\lambda_n} \right\} + \{\eta_n\} \qquad n = 1,\ldots,256$$

where $g_{xy}(\lambda)$ is the optical response of the spectrometric transducer,

$s(\lambda;\mathbf{l},\mathbf{a}) = \sum_{k=1}^{81} a_k \delta(\lambda - l_k)$ is the so-called idealized spectrum of input light, and $\{\eta_n\}$ is a sequence modeling the random errors in the data and the amplified spontaneous emission (ASE) noise caused by the laser sources. This is an adequate model for the DWDM measurements if the function $g_{sx}(\lambda)$ is an approximation of the shape of the laser light emission spectrum.

The *a priori* information about emission light of a laser is used for reconstruction of the idealized light spectrum $s(\lambda;\mathbf{l},\mathbf{a})$.

The continual re-calibration sub-procedure allows the measurement of the spectrum of laser emission in 1s time intervals to continually update parameters $\mathbf{p}_R$ of reconstruction sub-procedure.

The chosen operator of projection, mapping the idealized spectrum $s(\lambda;\mathbf{l},\mathbf{a})$ into the space of the data:

$$\{\hat{y}_n\} = G\left[s(\lambda;\mathbf{l},\mathbf{a});\mathbf{p}_G\right]$$

has been defined by the following operations:

$$x(\lambda) = \int_{-\infty}^{+\infty} g_{sx}(\lambda-\lambda')s(\lambda';\mathbf{l},\mathbf{a})\,d\lambda'$$

$$y(\lambda) = \int_{-\infty}^{+\infty} g_{xy}(\lambda-\lambda')\,x(\lambda')\,d\lambda'$$

$$\hat{y}_n = y(\lambda_n) \text{ for } n = 1,\ldots,N$$

The function $g_{xy}(\lambda)$ has been assumed to have the form of the Gauss function:

$$g_{xy}(\lambda) = \frac{1}{\sqrt{2\pi}\sigma_{xy}}\exp\left(-\frac{\lambda^2}{2\sigma_{xy}^2}\right)$$

Consequently, the vector of the parameters $\mathbf{p}_G$ of the operator G contains the discrete values of $g_{sx}(\lambda)$, shown in Fig. 11 and the parameter σ_{xy}, equal to the spectral bandwidth of the MM μOSA.

The chosen operator of reconstruction, transforming the data $\{\tilde{y}_n\}$ into an estimate $\hat{s}(\lambda)$ of $s(\lambda;\mathbf{l},\mathbf{a})$, :

$$\hat{s}(\lambda) = R\left[\{\tilde{y}_n\};\mathbf{p}_R\right]$$

is defined in the following way:

- a discrete estimate $\{\hat{x}_n\}$ of $x(\lambda)$ is found by means of the rational filter applied to the data $\{\tilde{y}_n\}$; and
- an estimate $\hat{s}(\lambda)$ of $s(\lambda;\mathbf{l},\mathbf{a})$ is computed by means of the spline-based Kalman filter applied to $\{\hat{x}_n\}$.

The vector $\mathbf{p}_R = [p_{R,1}\, p_{R,2} \ldots]^T$ of the parameters of the operator $\mathbf{R}$ contains the coefficients of the rational filter, as well as the discrete values of the function $g_{xx}(\lambda)$ and a regularization parameters required by the spline-based Kalman filter as described in in Ben Slima M., Morawski R. Z., Barwicz A.: "Kalman-filter-based Algorithms of Spectrophotometric Data Correction - Part II: Use of Splines for Approximation of Spectra", *IEEE Trans. Instrum. & Meas.*, Vol. 46, No. 3, June 1997, pp. 685-689.

The following operations are accomplished during the initial calibration:

- estimation of the coefficients of the rational filter using an optimization algorithm; and,
- estimation of the regularization parameter of the spline-based Kalman filter, using an optimization algorithm.

The update of coefficients of the rational filter is achieved during the continual re-calibration on the basis of the measured light emission spectrum of a laser.

Results of adaptive reconstruction and interpretation of telecommunication data obtained according to the present exemplary embodiment are shown in Fig. 12.

The following errors are defined to evaluate the exactitude of the present exemplary method:

- relative root-mean-square error (RRMSE)

$$\varepsilon_a = \frac{\|\mathbf{a}_{ex} - \mathbf{a}_{est}\|}{\|\mathbf{a}_{ex}\|}, \qquad \varepsilon_l = \frac{\|\mathbf{l}_{ex} - \mathbf{l}_{est}\|}{\|\mathbf{l}_{ex}\|}$$

- maximum absolute error (MAE)

$$\Delta_a = \max\{|\mathbf{a}_{ex} - \mathbf{a}_{est}|\}, \quad \Delta_a = \max\{|\mathbf{l}_{ex} - \mathbf{l}_{est}|\}$$

The errors of estimation of positions and heights of peaks, are:

$$\varepsilon_l = 2 \cdot 10^{-3}\,\%, \quad \Delta_l = 0.05\,\text{nm}; \quad \varepsilon_a = 1.3\,\%, \quad \Delta_l = 0.5\,\text{dBm};$$

4. Applicability and scope of the invention

The proposed procedure AI-RC may be applied in various light spectrum measuring instruments and systems, especially in miniaturized integrated spectrometers for *in situ* applications such as environmental probes, optical spectrum analyzers and optical performance monitors in telecommunication etc. The motivation for its application in a given measurement situation is founded on expected gains in performance and resolution such as the following examples:

- increased accuracy of spectrometric analyses accomplished by a given spectrometric system, resulting from correction of instrumental imperfections and reduced uncertainty of estimation of the parameters of measured spectra;
- possibility of automatic calibration of especially miniature integrated spectrometric devices during manufacturing process, taking into account their fabrication discrepancies;
- miniaturization and integration of light-spectrum-measurement related tools, resulting from the software compensation of their hardware imperfections and software replacement of some their functions; and
- reduced costs of spectrometric analyses, given the required accuracy, by replacing a high-resolution spectrometric devices with a functionally equivalent but low-resolution instrument.

As is evident to those of skill in the art, a known drawback to miniaturisation of spectral devices is that manufacturing at very small scales and light propagation through devices at those scales often highlights even small imperfections in the manufacturing processes and magnifies errors in manufacture. As such, a method of calibrating each device to correct for said imperfections would be extremely advantageous in some situations.

The exemplary embodiment of the invention, presented in section 3 is not intended to limit the applicability of AI-RC to absorption spectrophotometry and the monitoring of optical telecommunication channels. Neither is it intended to limit the variety of algorithms that may be used to embody the operations the procedure is composed of. On the contrary, the invention is intended to cover alternatives,

modifications and. Some practical options for methods embodying the operations of AI-RC are briefly characterized.

4.1. Optional forms of the operators of projection and reconstruction

The following mathematical models of the spectrometric data may be used for defining the operator G :

a) the stationary linear model:

$$y(\lambda) = \int_{-\infty}^{+\infty} g(\lambda - \lambda')\, s(\lambda'; \mathbf{l}, \mathbf{a})\, d\lambda'$$

b) the non-stationary linear model:

$$y(\lambda) = \int_{-\infty}^{+\infty} g(\lambda, \lambda')\, s(\lambda'; \mathbf{l}, \mathbf{a})\, d\lambda'$$

c) the non-linear model, e.g.:

$$y(\lambda) = \int_{-\infty}^{+\infty} g(\lambda, \lambda')\, F_s\left[s(\lambda'; \mathbf{l}, \mathbf{a})\right] d\lambda'$$

$$y(\lambda) = F_y\left[\int_{-\infty}^{+\infty} g(\lambda, \lambda')\, F_s\left[s(\lambda'; \mathbf{l}, \mathbf{a})\right] d\lambda'\right]$$

where $g(\lambda)$ and $g(\lambda, \lambda')$ are the apparatus functions of the spectrometric apparatus; F_s and F_y are non-linear functions.

The corresponding operators G may have the following forms:

a) the operator corresponding to the stationary linear model:

$$\hat{y}_n = \sum_{\nu} p_{G\,n,\nu} \int_{\lambda_\nu}^{\lambda_{\nu+1}} s(\lambda'; \mathbf{l}, \mathbf{a})\, d\lambda'$$

where $p_{G,\nu} = g\left(\frac{\lambda_{\nu+1} + \lambda_\nu}{2}\right) \Delta\lambda$;

b) the operator corresponding to the non-stationary linear model:

$$\hat{y}_n = \sum_{\nu} p_{G\,n,\nu} \int_{\lambda_\nu}^{\lambda_{\nu+1}} s(\lambda'; \mathbf{l}, \mathbf{a})\, d\lambda'$$

where $p_{G\,n,\nu} = g\left(\lambda_n, \frac{\lambda_{\nu+1} + \lambda_\nu}{2}\right) \Delta\lambda$;

c) the operator corresponding to the exemplary non-linear models:

$$\hat{y}_n = \sum_{\nu} p_{G\,n,\nu} \int_{\lambda_\nu}^{\lambda_{\nu+1}} F_s\left[s(\lambda';\mathbf{l},\mathbf{a})\right] d\lambda'$$

$$\hat{y}_n = F_y\left[\sum_{\nu} p_{G\,n,\nu} \int_{\lambda_\nu}^{\lambda_{\nu+1}} F_s\left[s(\lambda';\mathbf{l},\mathbf{a})\right] d\lambda'\right]$$

where $p_{G\,n,\nu} = g\left(\lambda_n, \frac{\lambda_{\nu+1}+\lambda_\nu}{2}\right)\Delta\lambda$.

4.2. Optional methods of signal reconstruction and interpretation

The following methods of signal reconstruction - deconvolution or generalized deconvolution - may be used for defining the operator R :

a) the original domain, numerical differentiation-based method defined in Morawski R. Z., Sokoł owski P.: "Application of Numerical Differentiation for Measurand Reconstruction", *Proc. 7th IMEKO-TC4 Int. Symp. Modern Electrical & Magnetic Measurements (Prague, Sept. 13-14, 1995)*, pp. 230-234;

b) the iterative methods of Jansson and Gold;

c) the spectrum-domain, Tikhonov-regularization-based method;

d) the cepstrum-domain, Tikhonov-regularization-based method defined in Kalinowska A., Morawski R. Z., Ł ubianka T.: "Incorpora- tion of the Positivity Constraint into a Cepstral Method of Measurand Reconstruction", *Proc. XIII-th IMEKO World Congress, (Torino, Italy, Sept. 5-9, 1994)*, pp. 429-434;

e) the original-domain, Tikhonov-regularization-based method with the positivity constraint imposed on the solution;

f) the Kalman-filter-based method with with the positivity constraint imposed on the solution;

g) the Kalman-filter-based method with spline-approximation of the solution;

h) the adjoint-operator method;

i) the entropy-based variational method;

j) the Volterra-series-based methods;

k) the rational-filter-based method; and,

l) the adaptive-rational-filter-based method.

Moreover, many other methods developed in the domain of chemometrics as described, for example, in Brown S. D., Bear Jr. R. S., Blank T. B.: "Chemometrics", *Anal. Chem.*, Vol. 64, No. 12, 1992, pp.22R-49R, and Brown S. D., Sum S. T., Despagne F.: "Chemometrics", *Anal. Chem.* Vol. 68, No. 12, 1995, pp. 21R-61R; telecommunications as described, for example, in Abreu E., Mitra S. K., Marchesani R.: "Non-minimum Phase Channel Equalization Using Non-causal Filters", *IEEE Trans. Signal Processing*, Vol. 45, No. 1, Jan. 1997, pp. 1-13 or seismology as described, for example, in Berkhout A. J.: *Seismic Migration*, Elsevier 1985 and image processing as described, for example, in numerous publications such as Gonsalves R. A., Nisenson P.:"HST Image Processing: An Overview of Algorithms for Image Restoration", *Proc. SPIE*, Vol. 1567, 1991, pp. 294-307 and Zerwakis M. E., Kwon T. M., "On the Application of Robust Functionals in Regularized Image Restoration",*Proc IEEE Int. Conf. Acoustics, Speech & Signal Process. - ICASSP'93 (Minneapolis MN, USA, April 27-30, 1993)*,Vol. 5, pp. 289-292 may be applied for this purpose.

The following methods are useful for determining the regularization parameters of the operator R :

a) the discrepancy principle with a pre-estimate of the variance of measurement errors in the data as described in Tikhonov A. N., Goncharsky A. V., Stepanov V. V., Yagola A. G.: *Numerical Methods for the Solution of Ill-Posed Problems*, Kluwer 1995;

b) the method of the L-curve as described in Hansen P. C., O'Leary D. P.: "The Use of the L-curve in the Regularization of the Discrete Ill-posed Problems", *SIAM J. Sci. Comput.*, Vol. 14, No. 6, 1993, pp. 1487-1503;

c) the method of additional set of calibration data as described in Szczeciń ski L., Morawski R. Z., Barwicz A.: "Numerical Correction of Spectrometric Data Using a Bilinear Operator of Measurand Reconstruction", *Proc. IEEE Instrum. & Meas. Technol. Conf. - IMTC'95 (Boston, MA, April 24-26, 1995)*, pp. 488-491.

4.3. Methods of calibration

It is often desirable to assume that the isolated peak $v_s(\lambda,l)$ has the following forms:

a) the Dirac distribution $\delta(\lambda)$ for all values of l;

b) a triangle whose width is constant or varying versus l;

c) a rectangle whose width is constant or varying versus l;

d) a Gauss function whose width is constant or varying versus l; and

e) a Lorenz function whose width is constant or varying versus l.

The following methods are useful in estimation of the apparatus function $g(\lambda)$:

a) smoothing approximation applied directly to the data $\{\tilde{y}_n^{cal}\}$ if the isolated peak $v_s(\lambda,l)$ is assumed to have the form the Dirac distribution $\delta(\lambda)$;

b) deconvolution of the data $\{\tilde{y}_n^{cal}\}$ with respect to $s(\lambda;\mathbf{l}^{cal},\mathbf{a}^{cal})$; and

c) subsequent use of deconvolution and smoothing approximation.

The following methods may be used for determining other parameters of the operator R :

a) a direct transformation of the parameters of the operator G ;

b) the minimization of any norm of the solution $\|\mathbf{p}_R\|$ under constraints imposed on another norm of the disrepancy $\left\|s\left(\lambda;\mathbf{l}^{cal},\mathbf{a}^{cal}\right)-\mathsf{R}\left[\{\tilde{y}_n^{cal}\};\mathbf{p}_R\right]\right\|$; and

c) the minimization of any norm of the disrepancy $\left\|s\left(\lambda;\mathbf{l}^{cal},\mathbf{a}^{cal}\right)-\mathsf{R}\left[\{\tilde{y}_n^{cal}\};\mathbf{p}_R\right]\right\|$ under constraints imposed on another norm of the solution $\|\mathbf{p}_R\|$.

4.4 Methods for estimation of the parameters of peaks

The following methods are useful for estimation of the magnitudes a of the peaks, given the estimates $\hat{\mathbf{l}}$ of their positions $\mathbf{l}$:

$$\hat{\mathbf{a}} = \arg_{\mathbf{a}} \inf\left\{\left\|\{\tilde{y}_n\}-G\left[s\left(\lambda;\hat{\mathbf{l}},\mathbf{a}\right);\mathbf{p}_G\right]\right\|_q \mid \mathbf{a}\in\mathsf{A}\right\}$$

or

$$\hat{\mathbf{a}} = \arg_{\mathbf{a}} \inf\left\{\left\|\hat{s}(\lambda)-s\left(\lambda;\hat{\mathbf{l}},\mathbf{a}\right)\right\|_q \mid \mathbf{a}\in\mathsf{A}\right\}$$

with **A** - being a set of feasible solutions; options: q=2 and $\mathbf{A} \subset R^k$; q=∞ and $\mathbf{A} \subset R^k$; q=2 and $\mathbf{A} \subset R_+^k$; q=∞ and $\mathbf{A} \subset R_+^k$. Some examples of algorithmic solutions are given in Morawski R. Z., Mię kina A., Barwicz A.: "Combined Use of Tikhonov Deconvolution and Curve Fitting for Spectrogram Interpretation", *Instrum. Science & Technology*, Vol. 24, No. 3, August 1996, pp. 155-167 and Morawski R. Z., Mię kina A., Barwicz A.: "The Use of Deconvolution and Iterative Optimization for Spectrogram Interpretation", *IEEE Trans. Instrum. & Meas., Vol. 47, No. 5, Oct.1997.* A particularly effective solution of the above optimization problem may be based on a non-stationary Kalman filter or an adaptive LMS algorithm is given in Ben Slima M., Morawski R. Z., Barwicz A.: "Kalman-filter-based Algorithms of Spectrophotometric Data Correction - Part II: Use of Splines for Approximation of Spectra", *IEEE Trans. Instrum. & Meas.*, Vol. 46, No. 3, June 1997, pp. 685-689.

Optionally, the methods for estimation of the magnitudes **a** are used for iterative correction of the estimates of the magnitudes **a** and positions **l** of the peaks interchangeably with the following methods:

$$\hat{\mathbf{l}} = \arg_{\mathbf{l}} \inf\left\{ \left\| \{\tilde{y}_n\} - G\left[s(\lambda;\mathbf{l},\hat{\mathbf{a}}); \mathbf{p}_G \right] \right\|_q \mid \mathbf{l} \in \mathbf{L} \right\}$$

or

$$\hat{\mathbf{l}} = \arg_{\mathbf{l}} \inf\left\{ \left\| \hat{s}(\lambda) - s(\lambda;\mathbf{l},\hat{\mathbf{a}}) \right\|_q \mid \mathbf{l} \in \mathbf{L} \right\}$$

with **L** being a set of feasible solutions; options: q=2 and $\mathbf{L} \subset R^k$; q=∞ and $\mathbf{L} \subset R^k$; q=2 and $\mathbf{L} \subset R_+^k$; q=∞ and $\mathbf{L} \subset R_+^k$.

4.5. Methods for pre-processing of the spectrometric data

The following methods are useful for normalization of the data:

a) the linear or nonlinear transformation of the λ-axis, aimed at diminishing the non-stationarity effects in the data;

b) the linear or nonlinear transformation of the *y*-axis, aimed at diminishing the non-linearity effects in the data; and

c) the linear or nonlinear transformation of the λ-axis and y-axis, aimed at diminishing the non-stationarity and non-linearity effects in the data.

The following methods are useful for smoothing the data:

a) the linear, FIR-type or IIR-type, filtering;

b) the median filtering;

c) the smoothing approximation by cubic splines; and

d) the deconvolution with respect to an identity operator.

Standard methods for baseline correction useful with the present invention are described in Brame E. G., Grasselli J., *Infrared and Raman Spectroscopy*, Marcel Dekker 1976 and in ASTM 1987. (American Society for Testing and Materials): *Annual Book of ASTM Standards* 1987.

Numerous other embodiments may be envisaged without departing from the spirit or scope of the invention.

What is claimed is:

1. A method of adaptive interpretation of spectrometric data combined with re-calibration for use with a spectrometric apparatus including transducer elements and comprising the steps of:

a) initially calibrating the spectrometric apparatus providing spectrometric data;

b) at intervals automatically re-calibrating the apparatus absent physical tuning of individual transducer elements in isolation by the steps of:

- providing light from a reference light source to the apparatus,
- acquiring auxiliary reference data relating to the detected light from the reference light source, and
- computing updated results of calibration based on the auxiliary reference data;

c) sensing a spectrum of light $\{x_n\}$ with the spectrometric apparatus to provide spectrometric data $\{\tilde{y}_n\}$ representative of the spectrum of light $\{x_n\}$;

d) adaptively determining an estimate $\{\hat{s}_n\}$ of an idealized spectrum $\{s_n\}$ related to the spectrum of light $\{x_n\}$ based on the spectrometric data $\{\tilde{y}_n\}$ and updated results of calibration; and,

e) adaptively estimating positions $l_1, l_2, \ldots$ and magnitudes $a_1, a_2, \ldots$ of peaks composing the spectrum of light $\{x_n\}$ on the basis of the estimate $\{\hat{s}_n\}$.

2. The method of claim 1 wherein the step (b) of recalibrating involves updating the results of a previous calibration absent physical modification and adjustment of the sensor elements.

3. The method of claim 1 wherein the step (a) comprises the steps of:

a1) selecting a form of peaks within the idealized spectrum $\{s_n\}$;

a2) choosing the form of the operator R for reconstruction of the idealized spectrum: $\{\hat{s}_n\}=\mathsf{R}\,[\{\tilde{y}_n\};\mathbf{p}_R\,]$, where $\mathbf{p}_R$ is a vector of the parameters, the form selected in dependence upon the selected form of the peaks;

a3) choosing rules for adaptation of the parameters $\mathbf{p}_R$ to selected features $F_1, F_2, \ldots$ of the data $\{\tilde{y}_n\}$ on the basis of the library of parameters $\{\mathbf{p}_R^{(j)} \mid j = 1,\ldots,J\}$ forming part of the calibration data determined during the step of initially calibrating and for updating during the step of re-calibrating;

a4) choosing a reference light signal for the step of initially calibrating: $\{x_n^{cal}(j)\}$ and related $\{s_n^{cal}(j)\}$ for $j=1,\ldots,J$;

a5) acquiring data $\{\tilde{y}_n^{cal}\}$ representative of $\{x_n^{cal}(j)\}$ for $j=1,\ldots,J$;

a6) pre-processing of the data $\{\tilde{y}_n^{cal}\}$;

a7) determination of the vectors of parameters $\mathbf{p}_R^{(j)}$ – on the basis of the triplets: $\{\tilde{y}_n^{cal}(j)\}$ $\{x_n^{cal}(j)\}$ and $\{s_n^{cal}(j)\}$ for $j=1,\ldots,J$;

a8) approximating a relationship between the parameters $\mathbf{p}_R$ and the features $F_1, F_2, \ldots$ controlling adaptation.

4. The method of claim 3 wherein the step (a6) comprises the step of:
acquiring *a priori* information relating to a pre-estimate of the variance of errors in the calibration data.

5. The method of claim 4 wherein the step (a6) comprises the steps of:
performing elimination of outliers,
performing baseline subtraction,
performing smoothing, and
normalizing the data.

6. The method of claim 3 wherein the step (a1) comprises the step of:
selecting a method of idealizing a spectrum indicative of a form of the peaks.

7. The method of claim 1 wherein the step (b) comprises the steps:

b1) choosing a reference light signals for re-calibration: $\{x_n^{recal}(j)\}$ and related $\{s_n^{recal}(j)\}$ for $j=1,\ldots,J$;

b2) acquiring data $\{\tilde{y}_n^{recal}\}$ representative of $\{x_n^{recal}(j)\}$ for $j=1,\ldots,J$;

b3) pre-processing the acquired data $\{\tilde{y}_n^{recal}\}$;

b4) updating of the vectors of parameters $\mathbf{p}_R^{(j)}$ on the basis of triplets: $\{\tilde{y}_n^{recal}(j)\}$, $\{x_n^{recal}(j)\}$ and $\{s_n^{recal}(j)\}$ for $j=1,\ldots,J$;

b5) updating the approximation of the relationship between the parameters $\mathbf{p}_R$ and the features $F_1, F_2, \ldots$ controlling the adaptation.

8. The method of claim 7 wherein the step (b3) comprises the step of:
acquiring *a priori* information relating to a pre-estimate of the variance of errors in the acquired data.

9. The method of claim 8 wherein the step (b3) comprises the steps of:
performing elimination of outliers,
performing baseline subtraction,
performing smoothing, and
normalizing the data.

10. The method of claim 1 wherein the step (d) comprises the steps of:

d1) pre-processing of $\{\tilde{y}_n\}$;

d2) computing an estimate of the idealized spectrum $\{s_n\}$ related to the spectrum under study $\{x_n\}$ on the basis of the data $\{\tilde{y}_n\}$, by means of the operator R with the parameters $\mathbf{p}_R$ adapted, at each consecutive step of data processing, to the features $F_1, F_2, \ldots$ – on the basis of the library of parameters, determined during initial calibration and updated during continual re-calibration.

11. The method of claim 10 wherein the step (d1) comprises the step of:

acquiring *a priori* information relating to accurate estimation of peak parameters.

12. The method of claim 11 wherein the step of acquiring *a priori* information comprises the step of:

acquiring *a priori* information relating to a pre-estimate of the variance of errors in the spectrometric data.

13. The method of claim 12 wherein the step (d1) comprises the steps of:

performing elimination of outliers,

performing baseline subtraction,

performing smoothing, and

normalizing the data.

14. The method of claim 1 wherein the step (e) comprises the steps of:

e1) pre-processing of the estimate $\{\hat{s}_n\}$ obtained in step (c);

e2) computing estimates of the positions and the magnitudes of the peaks within the first spectrum $\{x_n\}$.

15. The method of claim 14 wherein the estimated positions and magnitudes relate to positions and magnitudes within an idealised first spectrum based on the acquired spectrum, the updated calibration data, and operators derived therefrom.

16. The method of claim 15 wherein the step of (e1) comprises the step of:

acquiring *a priori* information relating to a number of peaks within the spectrometric data and an estimate of their widths.

17. The method of claim 16 wherein the step (e1) comprises the steps of:

performing elimination of outliers,

performing baseline subtraction,

performing smoothing, and

normalizing the data.

18. A spectrometric apparatus comprising:

transducer elements for sensing a spectrum of light $\{x_n\}$ with the spectrometric apparatus to provide spectrometric data $\{\tilde{y}_n\}$ representative of the spectrum of light $\{x_n\}$;

means for initially calibrating the spectrometric apparatus in response to a provided reference light to provide initial results of calibration;

means for automatically re-calibrating the apparatus in response to a provided reference light absent physical tuning of the transducer elements; and,

a processor for determining an estimate $\{\hat{s}_n\}$ of an idealized spectrum $\{s_n\}$ related to the first spectrum of light $\{x_n\}$ based on the spectrometric data $\{\tilde{y}_n\}$ and updated results of calibration and for estimating positions $l_1, l_2, \ldots$ and magnitudes $a_1, a_2, \ldots$ of peaks within the idealized spectrum $\{s_n\}$ based on the estimate $\{\hat{s}_n\}$.

19. A spectrometric apparatus comprising:

transducer elements for sensing a spectrum of light $\{x_n\}$ with the spectrometric apparatus to provide spectrometric data $\{\tilde{y}_n\}$ representative of the spectrum of light $\{x_n\}$; and,

means for initially calibrating the spectrometric apparatus in response to a provided reference light to provide initial results of calibration;

characterised by:

means for automatically re-calibrating the apparatus in response to a provided reference light absent physical tuning of the transducer elements

wherein during calibration of the spectrometric apparatus determination of parameters for use in reconstructing an idealised spectrum from data relating to light provided to the apparatus is performed.

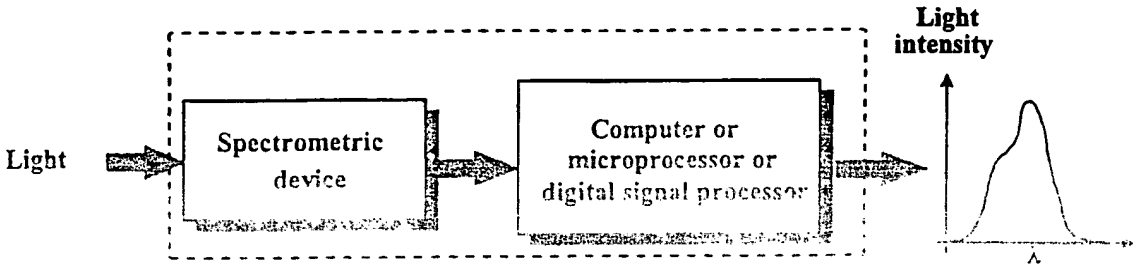

Light
Spectrometric device
Computer or microprocessor or digital signal processor
Light intensity
λ

Fig. 1

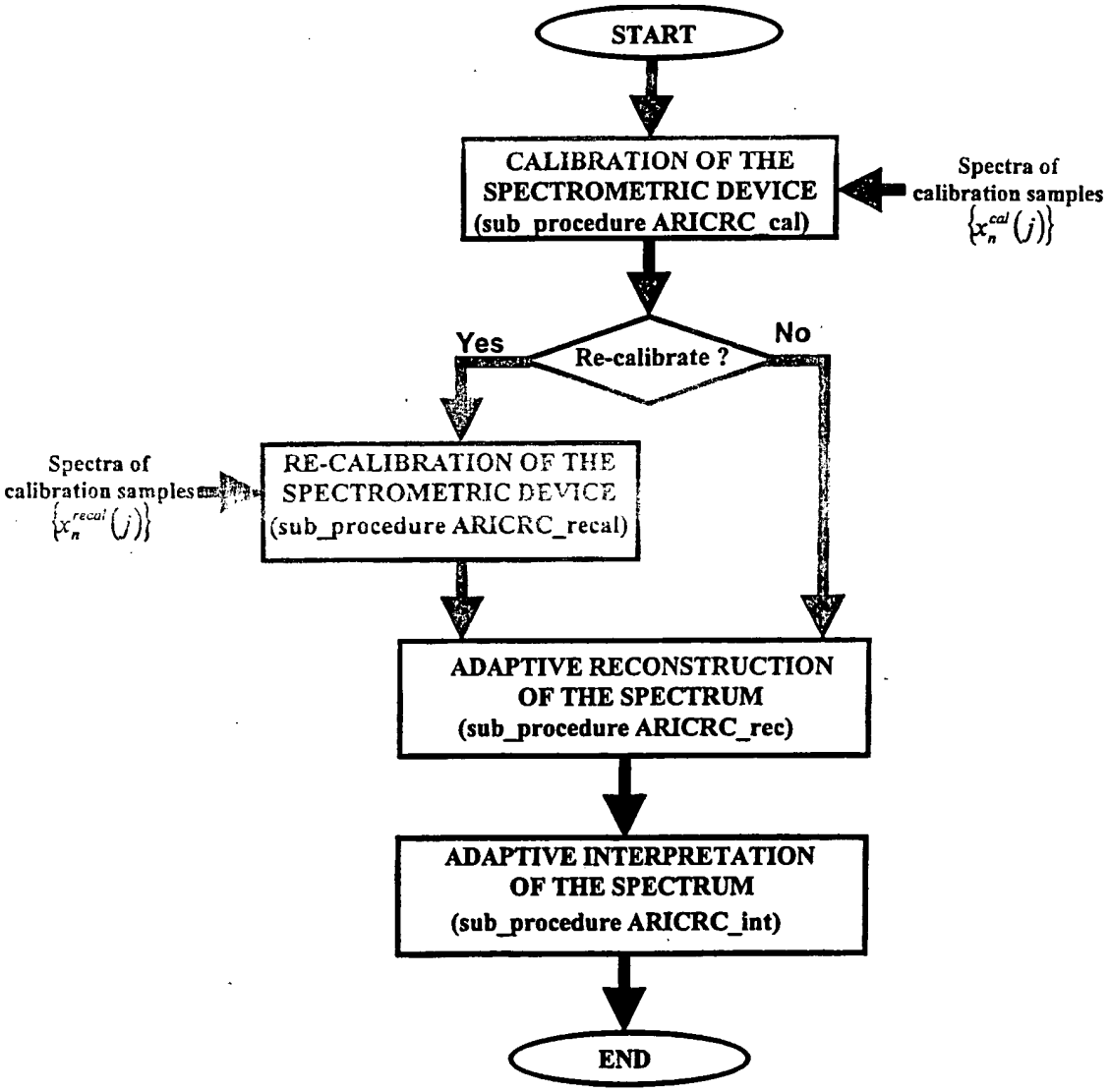

START
CALIBRATION OF THE SPECTROMETRIC DEVICE (sub_procedure ARICRC_cal)
Spectra of calibration samples $\{x_n^{cal}(j)\}$
Yes
Re-calibrate ?
No
Spectra of calibration samples $\{x_n^{recal}(j)\}$
RE-CALIBRATION OF THE SPECTROMETRIC DEVICE (sub_procedure ARICRC_recal)
ADAPTIVE RECONSTRUCTION OF THE SPECTRUM (sub_procedure ARICRC_rec)
ADAPTIVE INTERPRETATION OF THE SPECTRUM (sub_procedure ARICRC_int)
END

Fig. 2a

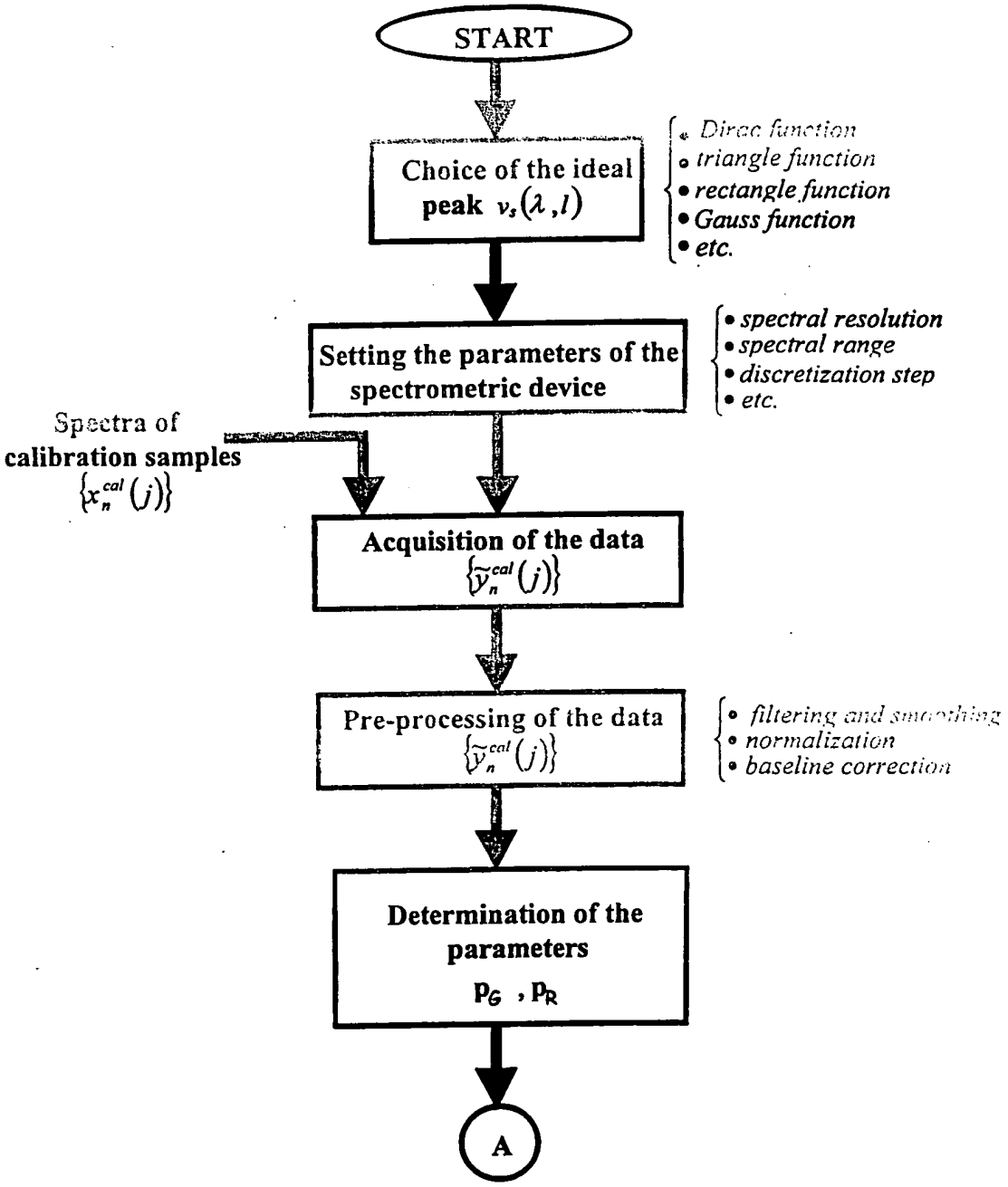

START
Choice of the ideal peak $v_s(\lambda, l)$
Dirac function
triangle function
rectangle function
Gauss function
etc.
Setting the parameters of the spectrometric device
spectral resolution
spectral range
discretization step
etc.
Spectra of calibration samples $\{x_n^{cal}(j)\}$
Acquisition of the data $\{\tilde{y}_n^{cal}(j)\}$
Pre-processing of the data $\{\tilde{y}_n^{cal}(j)\}$
filtering and smoothing
normalization
baseline correction
Determination of the parameters p_G , p_R
A

Fig. 2b

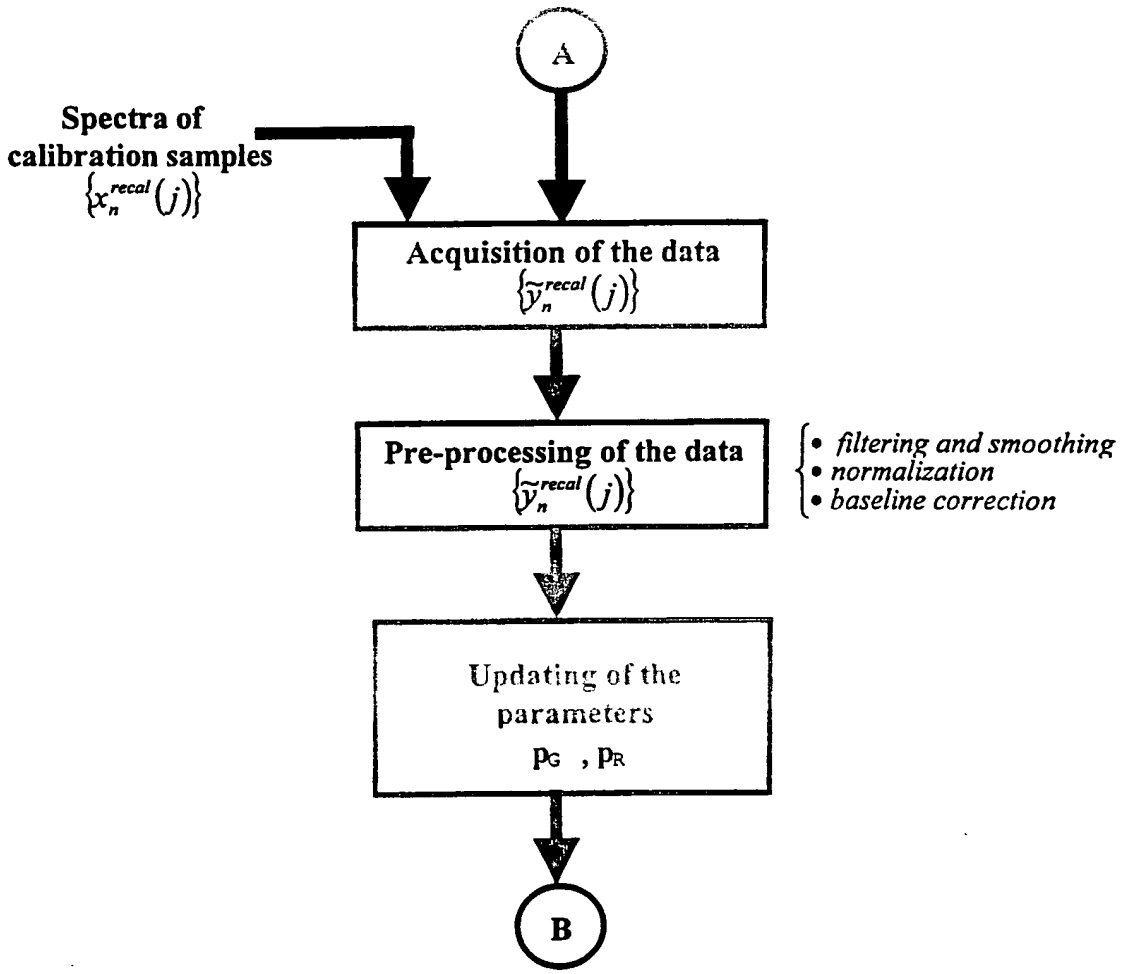

A
Spectra of calibration samples
$\{x_n^{recal}(j)\}$
Acquisition of the data
$\{\tilde{y}_n^{recal}(j)\}$
Pre-processing of the data
$\{\tilde{y}_n^{recal}(j)\}$
• filtering and smoothing
• normalization
• baseline correction
Updating of the parameters
p_G , p_R
B

Fig. 2c

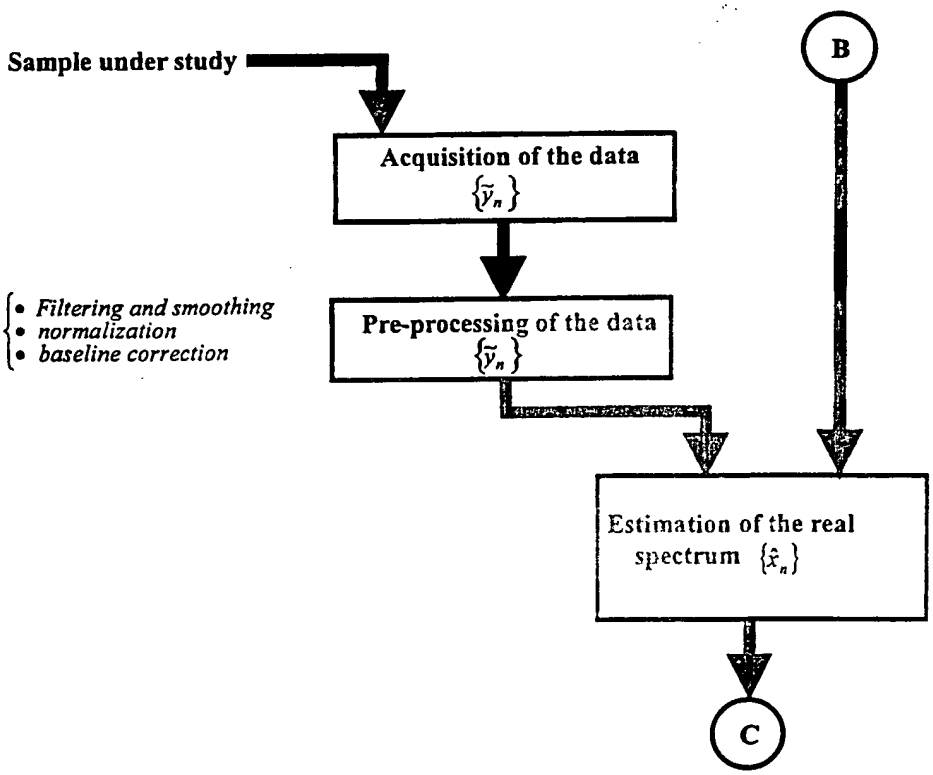

Sample under study
Acquisition of the data
$\{\tilde{y}_n\}$
• Filtering and smoothing
• normalization
• baseline correction
Pre-processing of the data
$\{\tilde{y}_n\}$
B
Estimation of the real spectrum $\{\hat{x}_n\}$
C

Fig. 2d

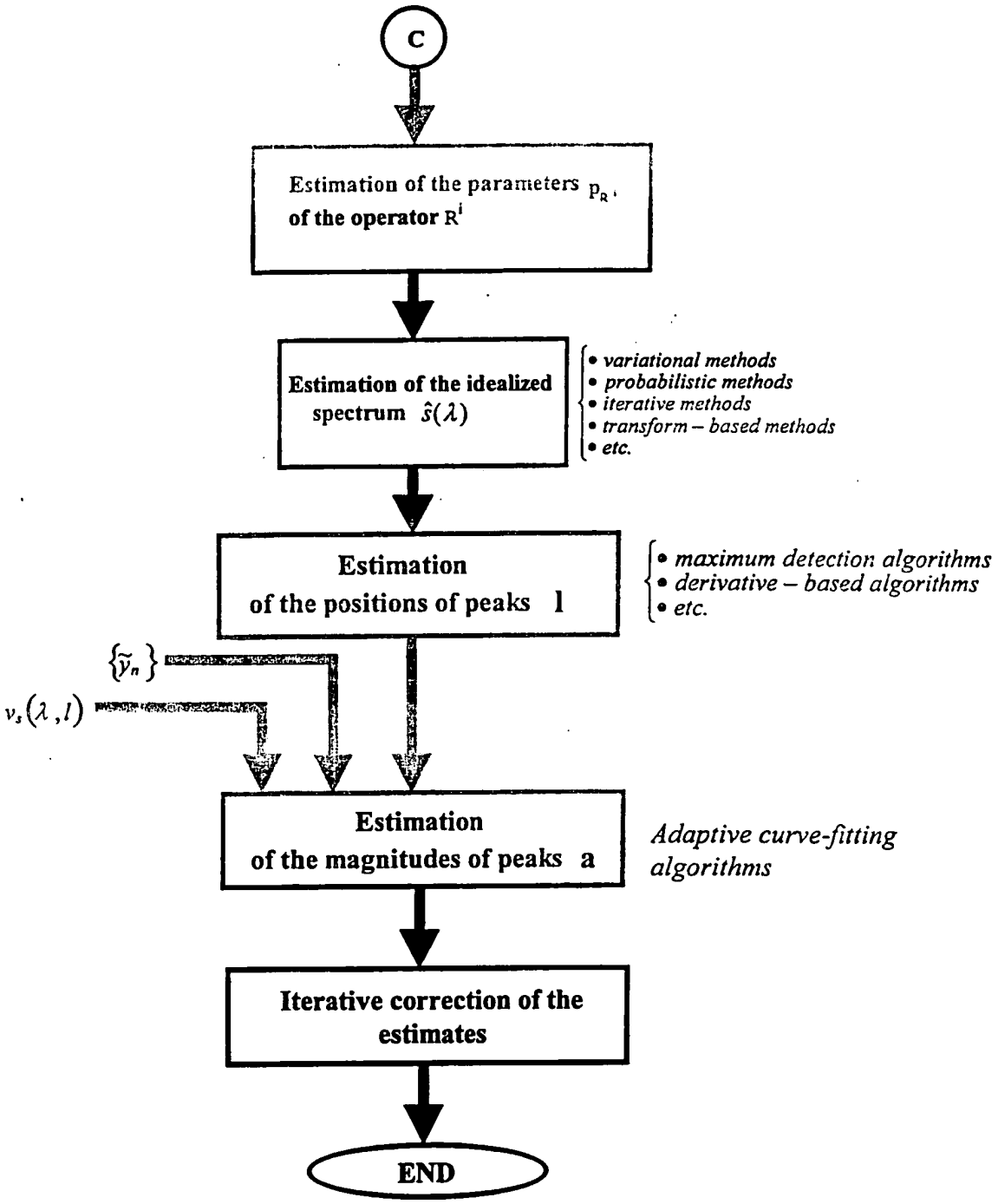

C
Estimation of the parameters p_R, of the operator R^i
Estimation of the idealized spectrum $\hat{s}(\lambda)$
• variational methods
• probabilistic methods
• iterative methods
• transform – based methods
• etc.
Estimation of the positions of peaks l
• maximum detection algorithms
• derivative – based algorithms
• etc.
$\{\tilde{y}_n\}$
$v_s(\lambda, l)$
Estimation of the magnitudes of peaks a
Adaptive curve-fitting algorithms
Iterative correction of the estimates
END

Fig. 2e

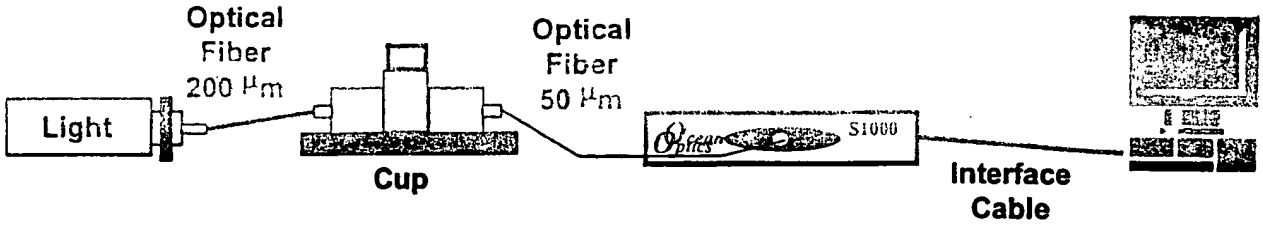

Optical
Fiber
200 μm
Light
Cup
Optical
Fiber
50 μm
S1000
Interface
Cable

Fig. 3

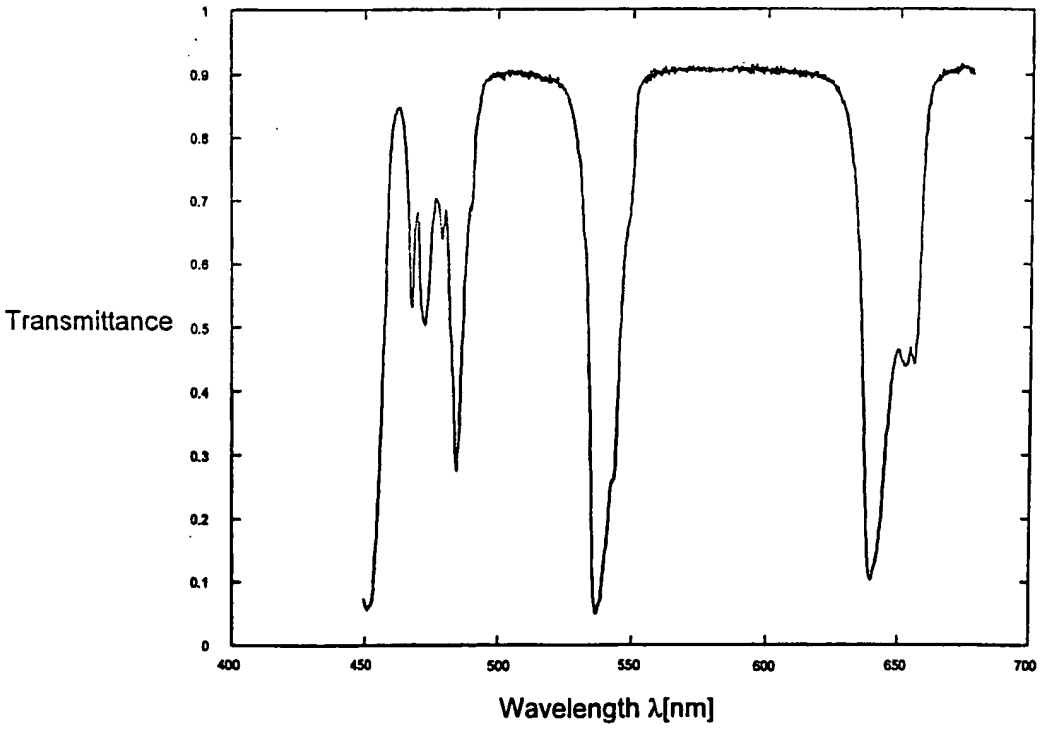

Transmittance
1
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
400
450
500
550
600
650
700
Wavelength λ[nm]

Fig. 4a

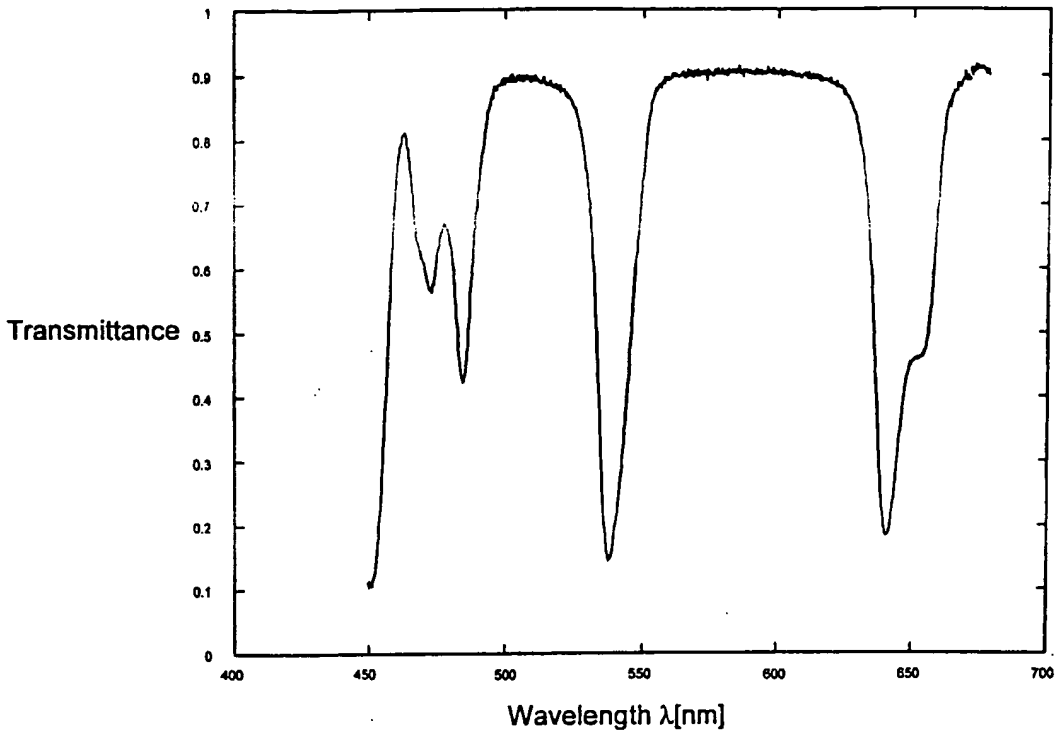

Transmittance
1
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
400
450
500
550
600
650
700
Wavelength λ[nm]

Fig. 4b

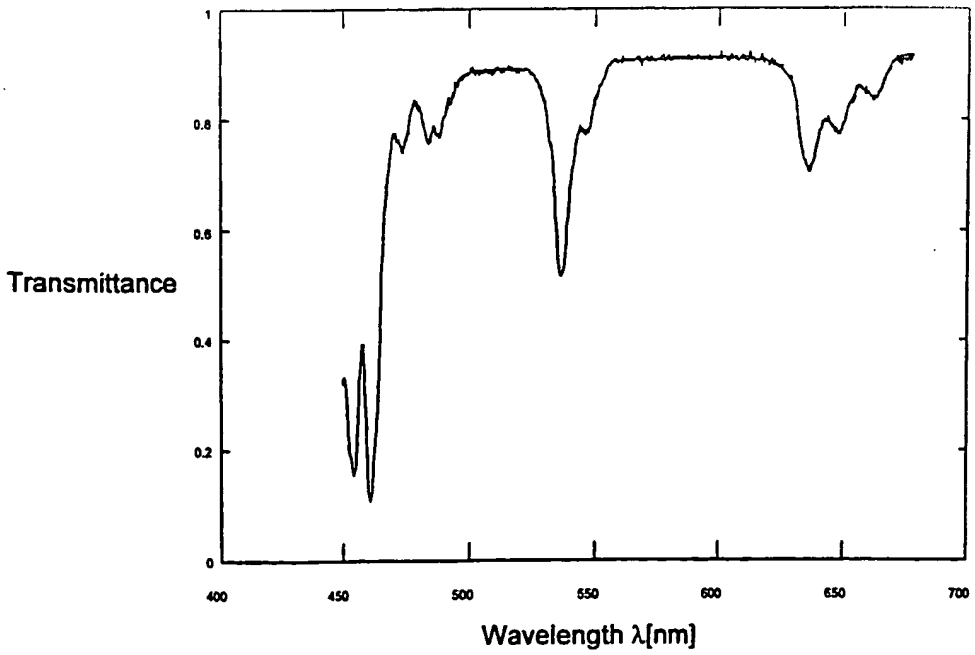

Transmittance
1
0.8
0.6
0.4
0.2
0
400
450
500
550
600
650
700
Wavelength λ[nm]

Fig. 5a

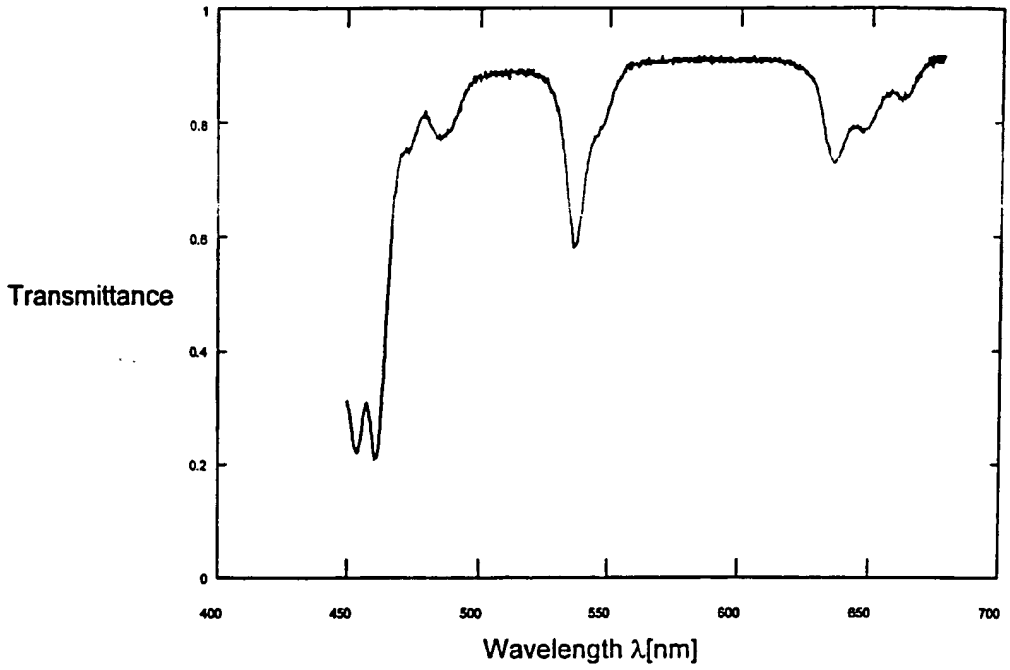

Transmittance
Wavelength λ[nm]

Fig. 5b

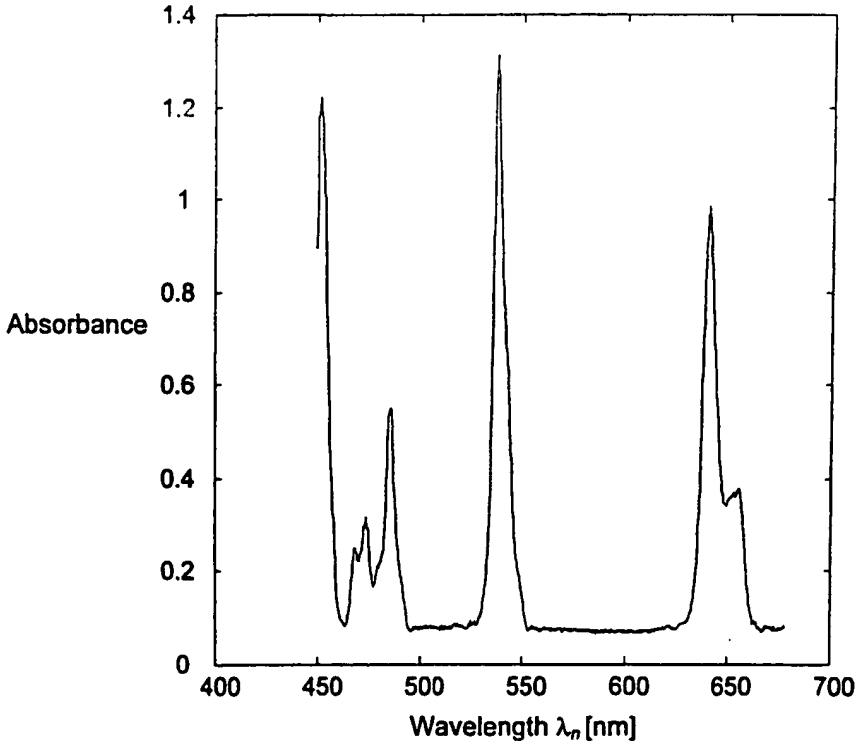

Absorbance
Wavelength λ_n [nm]

Fig. 6a

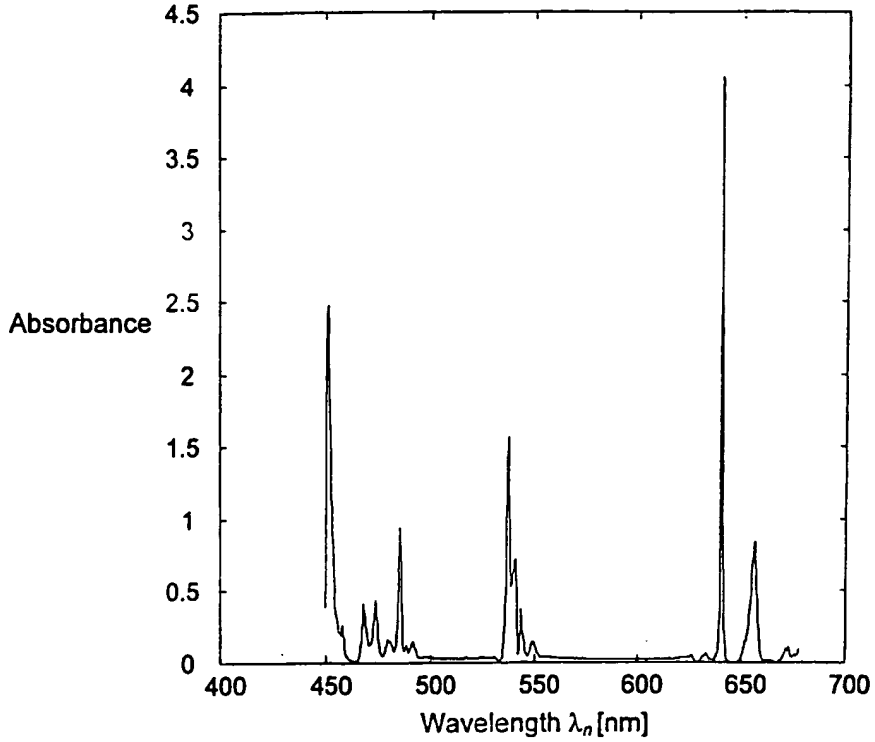

Absorbance
4.5
4
3.5
3
2.5
2
1.5
1
0.5
0
400
450
500
550
600
650
700
Wavelength λ_n [nm]

Fig. 6b

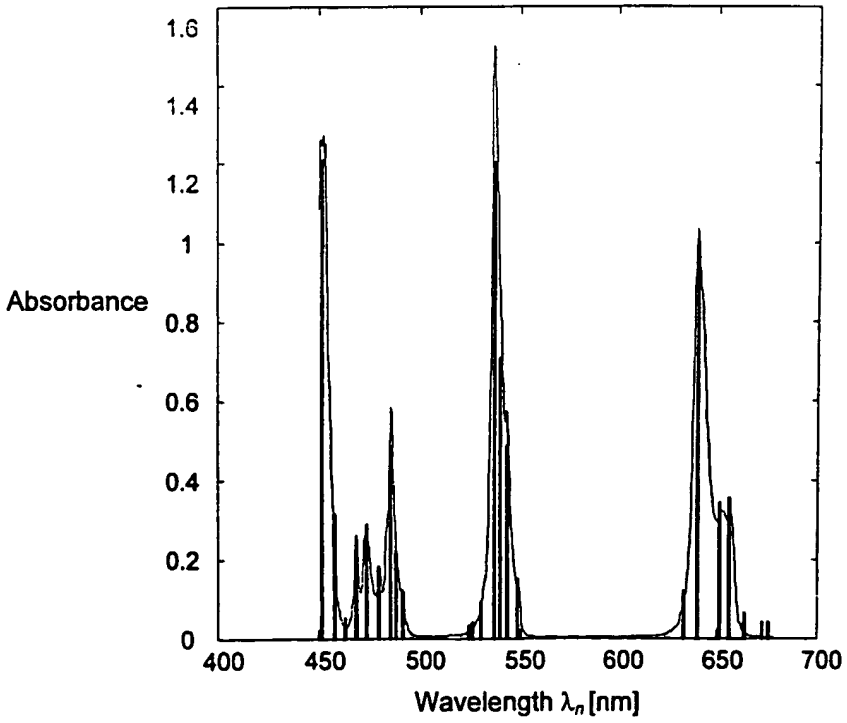

Absorbance
1.6
1.4
1.2
1
0.8
0.6
0.4
0.2
0
400
450
500
550
600
650
700
Wavelength λ_n [nm]

Fig. 7

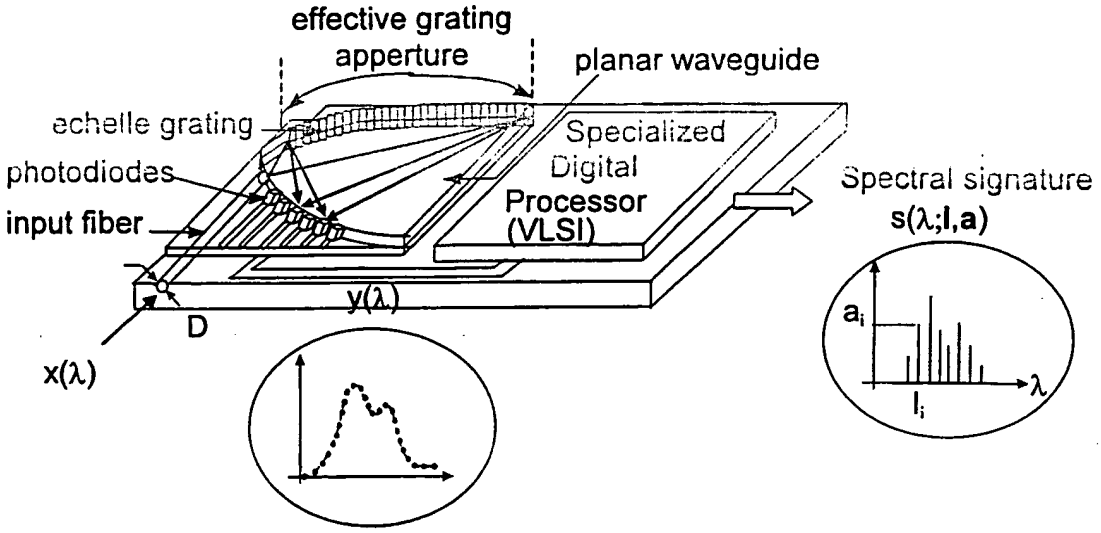

effective grating
apperture
planar waveguide
echelle grating
photodiodes
input fiber
Specialized
Digital
Processor
(VLSI)
Spectral signature
s(λ;I,a)
y(λ)
D
x(λ)
a_i
λ
I_i

Fig. 8

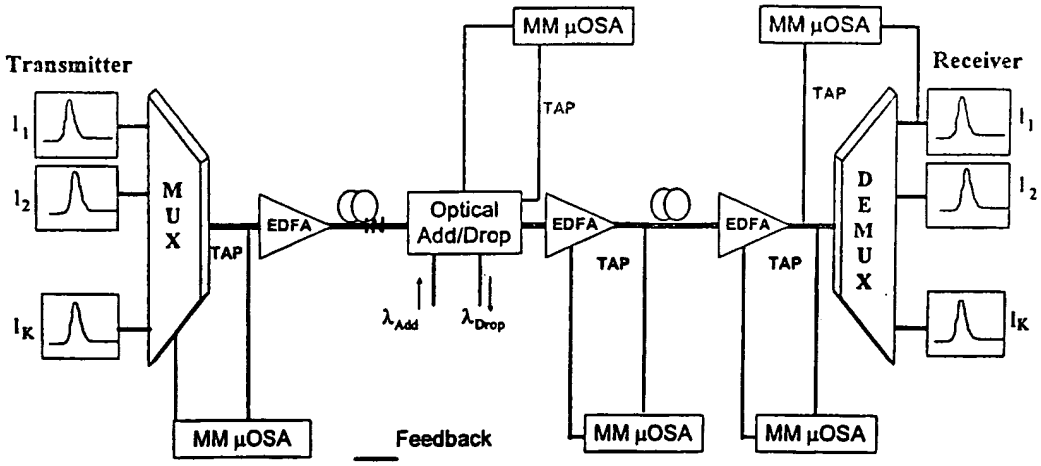

Transmitter
MM µOSA
MM µOSA
Receiver
TAP
TAP
I1
I2
IK
MUX
TAP
EDFA
Optical
Add/Drop
EDFA
EDFA
DEMUX
TAP
TAP
I1
I2
IK
λAdd
λDrop
MM µOSA
Feedback
MM µOSA
MM µOSA

Fig. 9

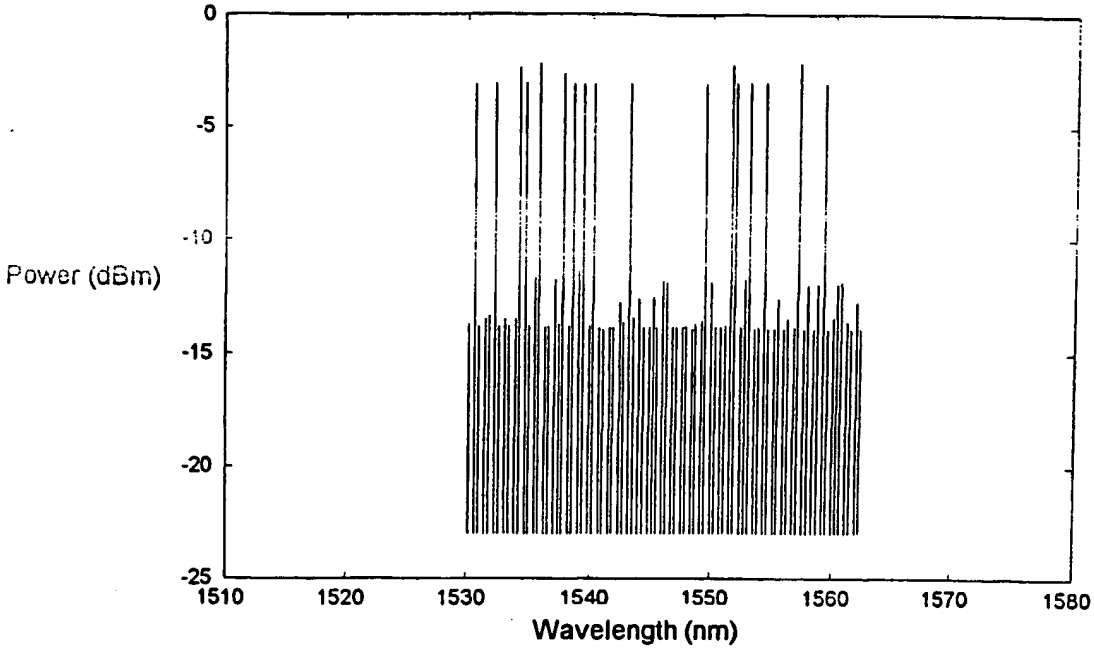


Fig. 10a

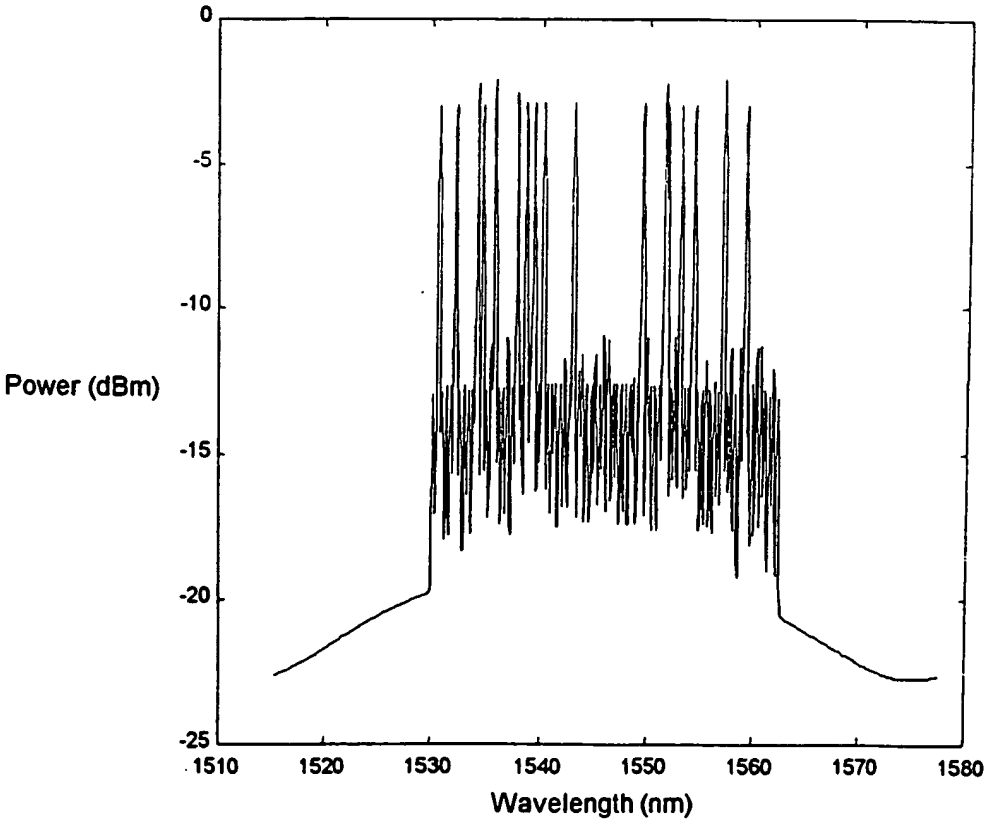


Fig. 10b

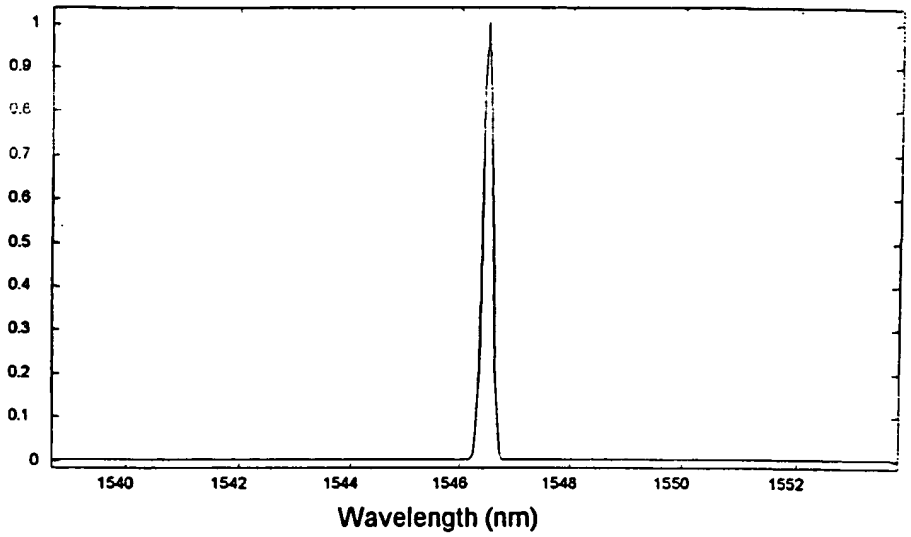

1
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
1540
1542
1544
1546
1548
1550
1552
Wavelength (nm)

Fig. 11

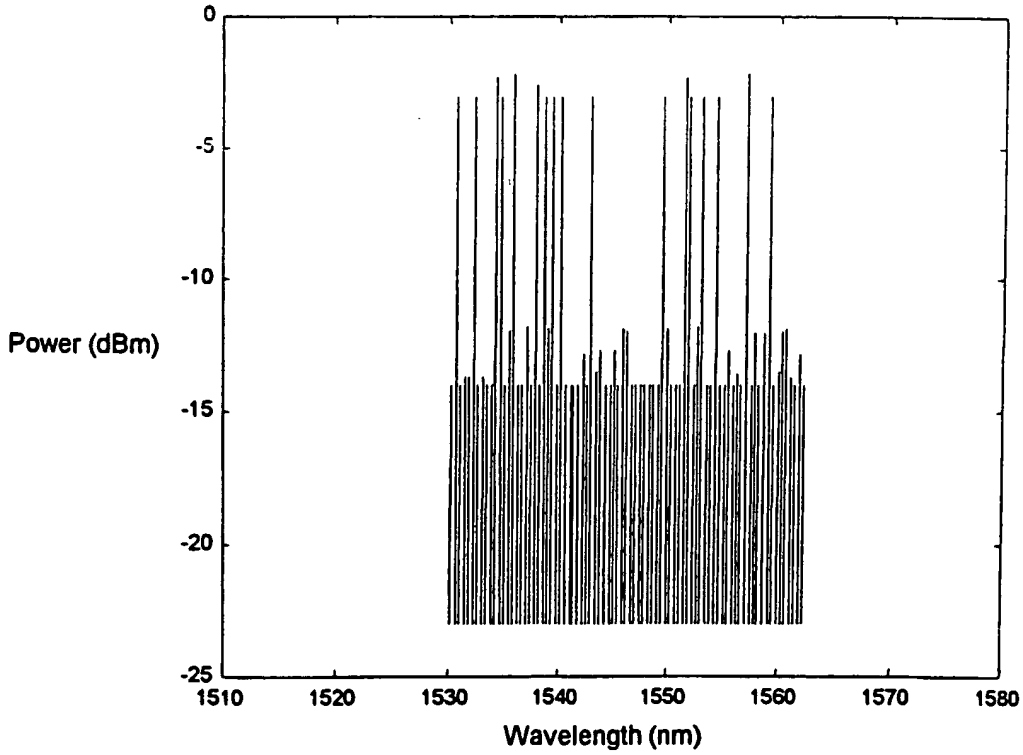

0
-5
-10
-15
-20
-25
Power (dBm)
1510
1520
1530
1540
1550
1560
1570
1580
Wavelength (nm)

Fig. 12

INTERNATIONAL SEARCH REPORT

Int tional Application No
PCT/CA 00/00583

A. CLASSIFICATION OF SUBJECT MATTER
IPC 7 G01J3/28 G01N21/27

According to International Patent Classification (IPC) or to both national classification and IPC

B. FIELDS SEARCHED

Minimum documentation searched (classification system followed by classification symbols)
IPC 7 G01J G01N

Documentation searched other than minimum documentation to the extent that such documents are included in the fields searched

Electronic data base consulted during the international search (name of data base and, where practical, search terms used)

EPO-Internal, WPI Data, PAJ

C. DOCUMENTS CONSIDERED TO BE RELEVANT

Category *	Citation of document, with indication, where appropriate, of the relevant passages	Relevant to claim No.
X	WO 98 53284 A (BARWICZ ANDRZEJ ;SLIMA MOHAMED B (CA); MEASUREMENT MICROSYSTEMS A) 26 November 1998 (1998-11-26)	1-4,6-8, 10-12, 14-16, 18,19
Y	page 8, line 26 -page 9, line 11 page 14, line 11 - line 27 page 21, line 7 -page 32, line 8	5,9,13, 17

-/--

[X] Further documents are listed in the continuation of box C.

[X] Patent family members are listed in annex.

* Special categories of cited documents :

"A" document defining the general state of the art which is not considered to be of particular relevance

"E" earlier document but published on or after the international filing date

"L" document which may throw doubts on priority claim(s) or which is cited to establish the publication date of another citation or other special reason (as specified)

"O" document referring to an oral disclosure, use, exhibition or other means

"P" document published prior to the international filing date but later than the priority date claimed

"T" later document published after the international filing date or priority date and not in conflict with the application but cited to understand the principle or theory underlying the invention

"X" document of particular relevance; the claimed invention cannot be considered novel or cannot be considered to involve an inventive step when the document is taken alone

"Y" document of particular relevance; the claimed invention cannot be considered to involve an inventive step when the document is combined with one or more other such documents, such combination being obvious to a person skilled in the art.

"&" document member of the same patent family

Date of the actual completion of the international search	Date of mailing of the international search report
21 September 2000	29/09/2000

Name and mailing address of the ISA	Authorized officer
European Patent Office, P.B. 5818 Patentlaan 2 NL – 2280 HV Rijswijk Tel. (+31-70) 340-2040, Tx. 31 651 epo nl, Fax: (+31-70) 340-3016	Jacquin, J

INTERNATIONAL SEARCH REPORT

International Application No
PCT/CA 00/00583

C.(Continuation) DOCUMENTS CONSIDERED TO BE RELEVANT

Category *	Citation of document, with indication, where appropriate, of the relevant passages	Relevant to claim No.
Y	MORAWSKI R Z ET AL: "COMBINED USE OF TIKHONOV DECONVOLUTION AND CURVE FITTING FOR SPECTROGRAM INTERPRETATION" INSTRUMENTATION SCIENCE & TECHNOLOGY,US,J.E. WAMPLER, vol. 24, no. 3, 1 August 1996 (1996-08-01), pages 155-167, XP000593577 ISSN: 1073-9149 page 157, paragraph 2 -page 158	5,9,13, 17
Y	EP 0 560 006 A (PERKIN ELMER CORP) 15 September 1993 (1993-09-15)	1,2,18, 19
A	column 7, line 17 - line 33 column 14, line 57 -column 15, line 33	3,7,10, 14
Y	US 4 681 444 A (FERBER ALAN C ET AL) 21 July 1987 (1987-07-21) column 2, line 3 - line 9 column 4, line 42 - line 47	1,2,18, 19
A	US 5 040 889 A (KEANE THOMAS J) 20 August 1991 (1991-08-20) cited in the application column 6, line 13 -column 9, line 12	1,18,19

INTERNATIONAL SEARCH REPORT

Information on patent family members

Int tional Application No
PCT/CA 00/00583

Patent document cited in search report	Publication date	Patent family member(s)	Publication date
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EP 0560006 A	15-09-1993	US 5303165 A	12-0 [illegible]
		CA [illegible] A	[illegible]
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		DE 69315607 T	30-04-1998
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